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Evalution of two-body operator matrix elements in the unitary group approach

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Abstract. We extend in this paper the Weyl graphical method to the two-body operator matrix elements in the many-particle system. The evaluation is accomplished by a simple and efficient recursion scheme.

1. Introduction

The application of unitary group methods to the analysis of many-body problems has been studied in considerable depth since the pioneering work of Gelfand and Zetlin [1]. The general complex closed formula for the matrix elements E_{ij} $(i>j)$ between canonical Gelfand tableaux were obtained by Baird and Biedenharn [2], Nagel and Moshinsky [3]. Moshinsky and co-workers [4] further extended these results to nuclear physics. An excellent review of the use of the unitary-group approach up to 1970 is given by Louck [5]. Simplifications of the unitary group formulae were made by Harter [6] and Drake *et al* [7]. One of these is the jawbone counting formula for elementary generator matrix elements based on Weyl tableaux which are equivalent to the Gelfand tableaux. They also made some improvement over the methods developed by Racah in the calculation of atomic problems.

Recently, we have published a series of papers [8-11] to extend the above jawbone counting formula of $E_{i,i-1}$ so as to include the general generators E_{ij}. Thus, the suggestion of Holman and Biedenharn [12], namely that the complicated closed formulae for E_{ij} in Gelfand tableaux would be converted to extremely simple graphical formulae based on Weyl tableaux, have been realised. We have referred to the method as the Weyl graphical method. Its main characters are as follows: (i) the values of matrix elements are factorised as the products of a few factors expressed as the axial distances; (ii) the repeated commutative relations, $E_{\mu\nu}=E_{\mu,\mu\pm1}E_{\mu\pm1,\nu}-E_{\mu\pm1,\nu}E_{\mu,\mu\pm1}$, are avoided; (iii) the crux of the calculation is to determine the integer with a circle. When the integer is different from that which enters the same position in the other Weyl tableau, the integer must be surrounded by a circle. Furthermore, if the difference is greater than one, the intermediate integers must also be added into this box with circles. In fact, all these integers with circles are just the altered weights in the Gelfand tableaux after the action of a generator E_{ij}.

The problem of the direct evaluation of the two-body operator matrix is, as is well known, of physical utility due to the fact that any realistic Hamiltonian of a many-particle system may be expressed as a linear combination of products of the group generators E_{ij}. Recently, Kent and Schlesinger [13] have presented a derivation of closed-form algebraic expressions for the two-body operator matrix elements by means of the distinct row table (DRT), as a generalisation of an SU(2) based method of Shavitt [14–16].

In this paper, we shall describe a different recursive approach to the factorisation of the two-body operator matrix elements, based directly on many-column Weyl tableaux, by the same graphical technique presented in [8–10]. This new approach offers a new and simpler insight.

2. The Weyl graphical method for one-body operator matrix elements

Here we present a review of the basic aspects of the Weyl graphical method for one-body operator matrix elements. As a distinguishing feature of this method, all the numbers in the initial and final Weyl tableaux which undergo a change with the action of the generator are contained in circles. And when the difference between the corresponding numbers for the two tableaux is larger than one, the intermediate numbers must be added into the two boxes simultaneously, and also contained in circles. Thus the matrix element $\langle (m')|E_{ij}|(m)\rangle$ $(i>j)$ is non-zero if and only if there are $i-j$ circled numbers in both (m') and (m); furthermore, these circled numbers for (m) are $j, j+1, \ldots, i-1$ and those for (m') are $j+1, j+2, \ldots, i$. In the appendix of [8] the formula for the matrix elements is of the form

$$\langle (m_l)|E_{ij}|(m_h)|\rangle = \prod_{r=1}^{i-j-1} H_r \prod_{r=1}^{i-j} \left(\frac{a_r d_r}{b_r c_r}\right)^{1/2} \qquad i>j \tag{1}$$

where H_r is the reciprocal of the axial distance between the circled $j+r$ and the circled $j+r-1$ in (m_h), and the factors a_r to d_r can be determined from the axial distances between the circled $j+r-1$ and the boxes entered by other $j+r-1$ and $j+r$ in (m_h).

For convenience, we present an alternative form of (1), i.e.

$$\langle (m')|E_{ij}|(m)\rangle = \prod_{l=j}^{i-2} H_{l+1,l} \prod_{l=j}^{i-1} M'_{l+1,l} \qquad i>j \tag{2}$$

where the value of $H_{l+1,l}$ is the reciprocal of the axial distance between the circled $l+1$ and circled l in (m) (when the two circled numbers are in the same box the axial distance is assigned the value 1), and if the row number of circled $l+1$ is not larger than that of circled l, the value of $H_{l+1,l}$ will be positive; it is negative otherwise. The expression for the factor $M'_{l+1,l}$ in (2) can further decompose into multiplicative factors as follows:

$$M'_{l+1,l} = \prod_{t=1, t\neq n_l}^{N_0} M''_{l+1,l} \tag{3}$$

where N_0 is the total number of columns in (m) and the index t is assigned to the column order; n_l is the order of the column in which the circled l is entered; the value of $M''_{l+1,l}$ can be determined from the relative position between the number l, $l+1$ in the tth column and circled l in (m), and is expressed in a simplified formula shown in figure 1(a).

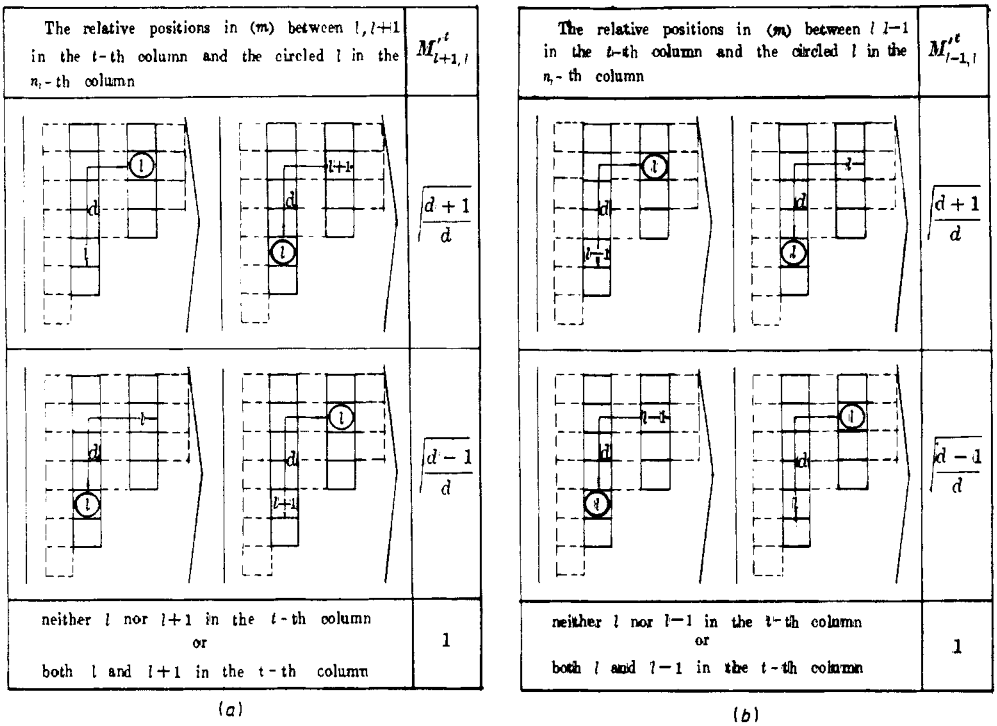


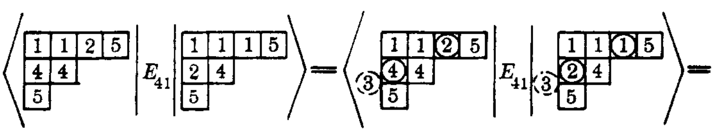
Figure 1. (a) The simplified formulae for $M_{l+1,l}'^{t}$ in the expression for lowering operator matrix elements. The simplified formulae for $M_{l-1,l}'^{t}$ in the expression for raising operator matrix elements.

The matrix element expression for the raising operator is also written down as

$$\langle (m')|E_{ji}|(m)\rangle = \prod_{l=j+2}^{i} H_{l-1,l} \prod_{l=j+1}^{i} M'_{l-1,l}$$

$$= \prod_{l=j+2}^{i} H_{l-1,l} \prod_{l=j+1}^{i} \prod_{t=1,t\neq n_l}^{N_0} M_{l-1,l}'^{t} \qquad i>j \tag{4}$$

where the value of $H_{l-1,l}$ is the reciprocal of the axial distance between the circled $l-1$ and circled l in (m), and if the row number of circled l is not larger than that of circled $l-1$ the value of $H_{l-1,l}$ will be positive, otherwise it is negative; the value of



$$= \prod_{l=1}^{2} H_{l+1,l} \prod_{l=1}^{3} M'_{l+1,l} = H_{2,1}H_{3,2}M'_{2,1}M'_{3,2}M'_{4,3} = (-\tfrac{1}{3})(1)(\sqrt{\tfrac{3}{2}}\cdot\sqrt{\tfrac{2}{1}}\cdot 1)(1\cdot 1\cdot 1)(\sqrt{\tfrac{2}{1}}\cdot 1\cdot 1)$$

$$= -\sqrt{\tfrac{2}{3}}$$

Figure 2. An example of the evaluation of lowering operator matrix elements by using the simplified formulae shown in figure 1(a).

$M_{l-1,l}^{tt}$ is determined from the relative positions of the number l, $l-1$ in the tth column and the circled l in (m), and is expressed in a simplified formula shown in figure 1(b). An example of this evaluation is shown in figure 2.

3. The Weyl graphical method for two-body operator matrix elements

The matrix elements of a two-body operator $E_{ij}E_{kl} = E_2E_1$ can be expressed in terms of one-body matrix elements as a sum of products:

$$\begin{aligned}\langle(m')|E_2E_1|(m)\rangle &= \sum_{(m'')} \langle(m')|E_2|(m'')\rangle\langle(m'')|E_1|(m)\rangle \\ &= \sum_{(m'')} \langle(m'')|E_2^{+}|(m')\rangle\langle(m'')|E_1|(m)\rangle \qquad (5)\end{aligned}$$

where the summation must extend over all intermediate states which have non-zero contributions.

This section will show how the required two-body operator matrix elements can be evaluated through an efficient iterative procedure in which the intermediate states need not be enumerated and summed individually.

From section 2 it follows immediately that an intermediate state carries with it the corresponding circled forms for both (m') and (m), which is the key to the solution of (5). The two-body operator matrix elements can be divided into two general types: one with overlapping index pairs (i, j) and (k, l) and the other with separate index pairs. We shall not treat the latter type because each (m') and (m) has only one circled form which can be easily obtained since the generators E_{ij} and E_{kl} operate within different parts of the Weyl basis tableaux. As for the overlapping type, it will only be necessary to consider the three cases: $E_{ji}E_{ji}$, $E_{ji}E_{ij}$ and $E_{ij}E_{ji}$.

3.1. *The case of* $\langle(m')|E_{ji}E_{ji}|(m)\rangle$ *with* $i>j$

In the case of the successive actions of two raising operators, the matrix elements will be zero unless there are $2(i-j)$ circled (or changed) numbers in both (m') and (m), which are $j, j, j+1, j+1, \ldots, i-1, i-1$ for (m') and $j+1, j+1, j+2, j+2, \ldots, i, i$ for (m). All these changed numbers can be determined by comparing the two tableaux. The key to the problem, however, is to determine the circled forms of (m') corresponding to $\langle(m'')|E_2^{+}|(m')\rangle$ and those of (m) corresponding to $\langle(m'')|E_1|(m)\rangle$. It is easy to understand that one of the two changed k in a single tableau would be associated with E_1, and the other would be associated with E_2. When the two k are in the same row, the assigning to one-body operators is unique and definite by virtue of the requirement that intermediate states must be standard Weyl tableaux. Nevertheless, when two k are neither in the same column nor in the same row, two ways of assigning—(1) and (2)—exist because each changed k may be associated with E_1 or E_2.

Here we define the two possible level circled forms for both (m) and (m') as follows.

Level circled form (1). For (m'), the upper right of the two changed $k+1$ is assigned to E_2^{+} and explicitly contained in a circle; for (m), the lower left of the two changed k is assigned to E_1 and explicitly contained in a circle.

Level circled form (2). For (m'), the lower left of the two changed $k+1$ is explicitly contained in a circle; for (m), the upper right of the two changed k is explicitly contained in a circle.

Thus, the graphical representations of the circled forms of (m') for $\langle(m'')|E_2^+|(m')\rangle$ and the circled forms of (m) for $\langle(m'')|E_1|(m)\rangle$ can be established in the following steps. First, for each of the two tableaux (m') and (m), all the level circled forms are listed out successively from level j to level i with forms (1) on the left and (2) on the right. When there is only one form in a level, it is classified as form (1) in this paper. In the k-level circled forms, all numbers k (with or without a circle) are written out (if k is added into a box as an intermediate number, the original number in this box, which must be contained in a circle, is also written out). Second, only two adjacent level circled forms which can match into a standard sub-tableau of an intermediate state after the change of the circled numbers, are linked with a line. Thus a single circled form of (m) or (m') is represented by a traverse from level j to level i successively along the existing lines in the graphical representation of (m) or (m'), respectively. It is worth noting that, under the above definition of level circled forms, the linkage between the levels k and $k+1$ in the graphical representation of (m') is the same as that between the levels $k+1$ and $k+2$ in the representation of (m). Hence the two corresponding traverses in the two representations refer to the two circled forms for $\langle(m'')|E_2^+|(m')\rangle$ and $\langle(m'')|E_1|(m)\rangle$ associated with a definite intermediate state (m'').

Furthermore, it is seen that each line between adjacent levels in the representation of (m') associates with definite factors in the expression of $\langle(m'')|E_2^+|(m')\rangle$. In the case that E_2^+ is a lowering operator, the line between levels $i-1$ and i is associated with the factor of $M'_{i,i-1}$, and the line between levels k and $k+1$ ($k=j, j+1, \ldots, i-2$) is associated with the two factors $H_{k+1,k}$ and $M'_{k+1,k}$. Similarly, each line between adjacent levels in the representation for (m) is associated with the definite factors in the expression for $\langle(m'')|E_1|(m)\rangle$. In the case of E_1 being a raising operator, the line between levels j and $j+1$ determines $M'_{j,j+1}$, and the line between levels k and $k+1$ ($k=j+1, j+2, \ldots, i-1$) determines $H_{k,k+1}$ and $M'_{k,k+1}$. Finally, we multiply the factors in the graphical representation of (m) by the factors associated with the corresponding line in the representation of (m') to obtain the combined factors $F(k)_{pq}$, where k is the larger of the two level numbers to which the line connects; the subscript p refers to the $k-1$th-level circled form number to which the line connects and q refers to the kth-level circled form number. In such a way, we establish the recursive graph, see figure 3, in which the level circled forms are replaced by nodes, and the level $i+1$ is added due to fact that the linkage between levels $i-1$ and i for (m') would correspond to the linkage between levels i and $i+1$ for (m).

In the recursive graph, there is a combined factor $F(k)_{pq}$ ($p, q=1, 2$) associated with each line. And there is a value $M(k)_t$ ($t=1, 2$) associated with each node, where subscript t also refers to the level circled form number and k refers to the level number. The recursive evaluation of the sum of (5) is carried out from levels j to $i+1$, in the form

$$\begin{aligned} &M(j)_1 = 1 \\ &M(k)_t = \sum_{t'} M(k-1)_{t'} \cdot F(k)_{t't} \qquad k=j+1, \ldots, i+1 \quad t=1,2. \\ &\langle(m')|E_{ji}E_{ji}|(m)\rangle = M(i+1)_1 \end{aligned} \tag{6}$$

where the summation t' extends over the nodes of level $k-1$, which are connected with the node of $M(k)_t$ by lines. It is seen that this recursive evaluation takes advantage of the common factors of the different intermediate states, and thus has avoided a

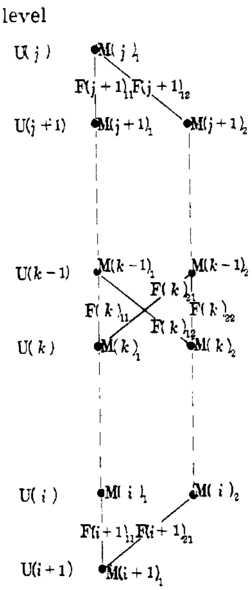


Figure 3. The formally recursive graph of matrix elements $\langle(m')|E_{ji}E_{ji}|(m)\rangle$.

summation over all these states individually, greatly simplifying and speeding up the computation. An example for this case is shown in figure 4.

3.2. *The case of* $\langle(m')|E_{ji}E_{ij}|(m)\rangle$

In this case both E_1 and E_2^+ are the lowering operator E_{ij}. Obviously, there should be $i-j$ circled numbers, $j, j+1, \ldots, i-1$, in every circled form of both (m') and (m). There is an important difference between this case and that in subsection 3.1. All these circled numbers may not be obtained by simple comparison between the two tableaux, as the action of a lowering operator is followed by a raising operator. Only some of these can be obtained and assigned definitely to E_1 to E_2^+ by this comparison. (These definite level circled forms are classified to form (1).) Thus, a different approach to finding out these hidden circled numbers is necessary. It is worth noting that these hidden circled numbers are the same for both (m) and (m'), and that the same hidden circled number is in the same position for the two tableaux. There are at most N_0 possible positions for one hidden circled k in (m') or (m), namely the last box in each column of the k-level sub-Weyl tableau. If the number in the last box is other than k, the hidden circled k is added into the box as the intermediate number (see section 2). Naturally, the level circled form number for both (m') and (m) is defined in the same way as the column order where the circled k is entered. Formally, there can be N_0 circled forms of level k; however there may be fewer forms in an actual calculation for two reasons: first, when several k are in the same row, only one can be contained in a circle by virtue of the rightmost requirement for the standard Weyl tableaux (m''); second, when the hidden circled k is added into a box as an intermediate number, the original number in this box must also be contained in a circle. Besides, there are some other differences between the cases of subsections 3.1 and 3.2. Now, the linkage between levels k and $k+1$ in the representation for (m') corresponds to that in the representation for (m), so the merging to the recursive graph is slightly different in

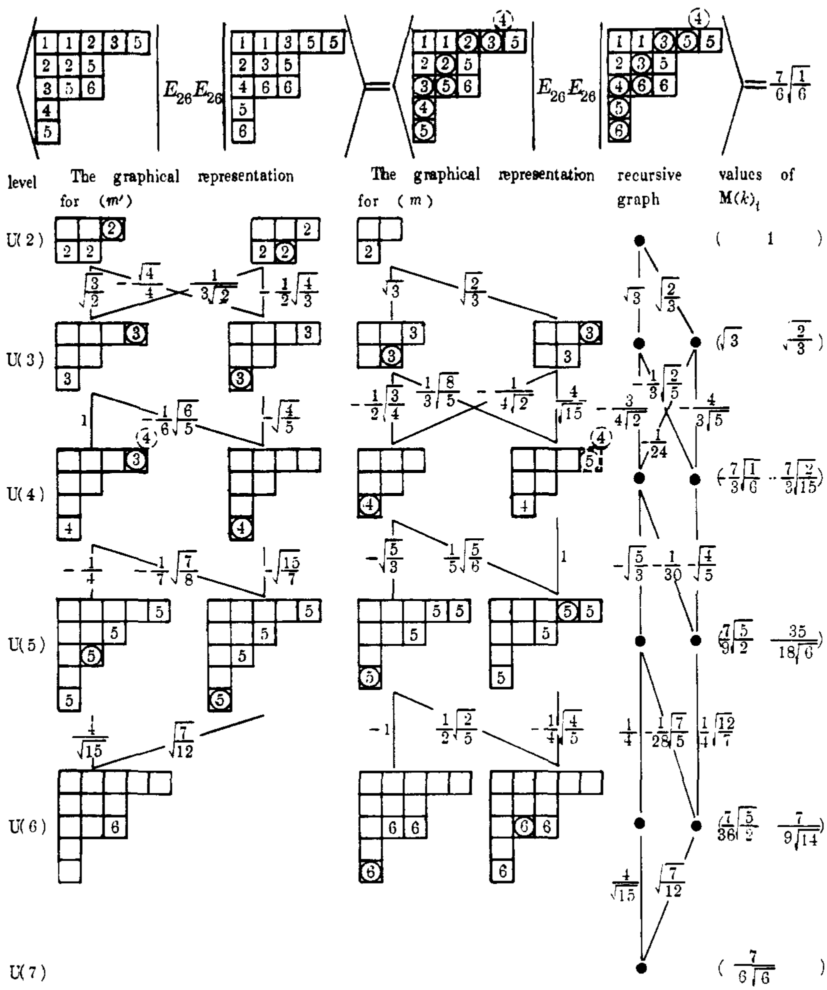


Figure 4. An example of the recursive evaluation of the matrix elements $\langle(m')|E_{ji}E_{ji}|(m)\rangle$.

that level $i+1$ is not needed. The desired matrix element value is just the value $M(i)_1$. The similar recursive formulae are

$$\begin{aligned} &M(j)_t = 1 \qquad t = 1, 2, \ldots \\ &M(k)_t = \sum_{t'} M(k-1)_{t'} F(k)_{t't} \qquad k = j+1, \ldots, i \quad t = 1, 2, \ldots \\ &\langle(m')|E_{ji}E_{ij}|(m)\rangle = M(i)_1. \end{aligned} \tag{7}$$

An example of this case is given in figure 5.

3.3. *The case of $\langle(m')|E_{ij}E_{ji}|(m)\rangle$*

In this case, both E_1 and E_2^+ are raising operators. So the treatment parallels that of the case in subsection 3.2 except for the possible positions for hidden circled k. When the number in the last box of a column in the k-level sub-Weyl tableau is other than k, the hidden circled k should be added into the next box (not belonging to the k-level sub-Weyl tableau) as an intermediate number. Of course, the original number in this

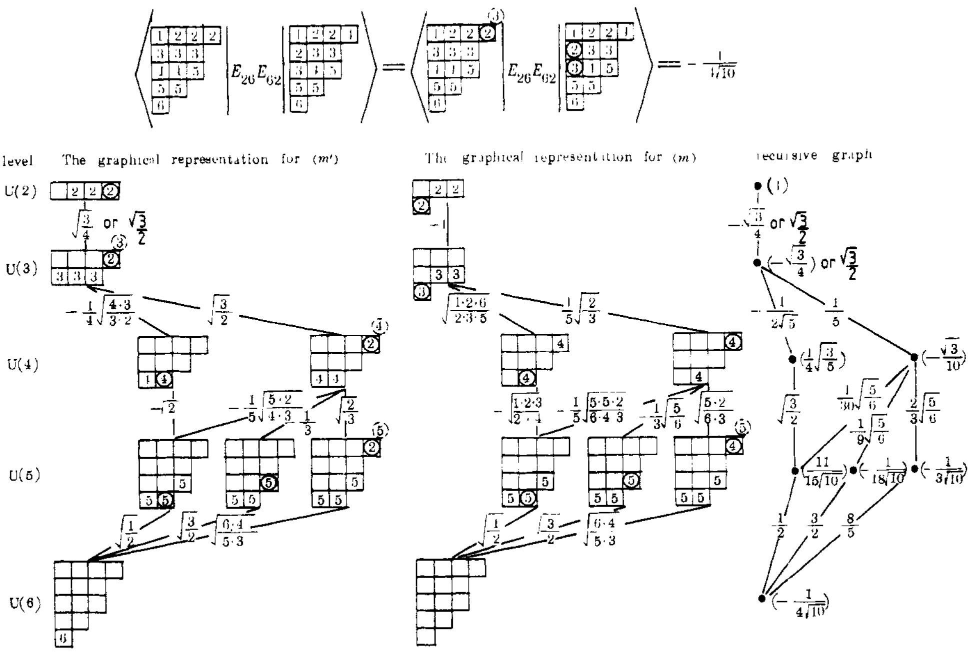


Figure 5. An example of the recursive evaluation of the matrix elements $\langle (m')|E_{ji}E_{ij}|(m)\rangle$. The values in parentheses in the recursive graph are the values of $M(k)_t$.

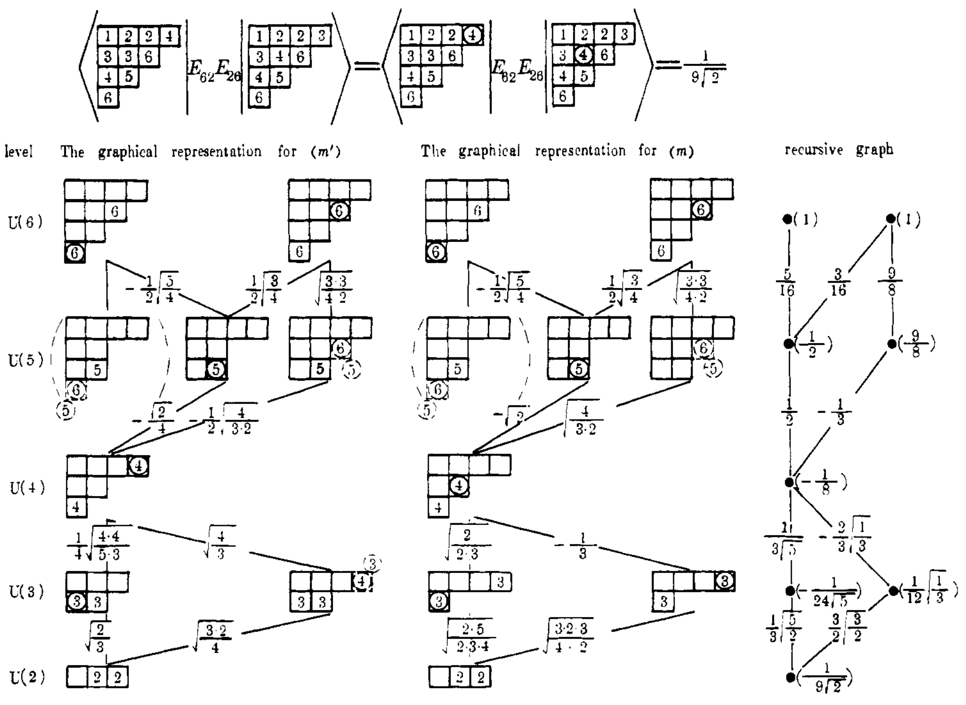


Figure 6. An example of the recursive evaluation of the matrix elements $\langle (m')|E_{ij}E_{ji}|(m)\rangle$. There is no line connecting the level circled form in broken parentheses to the next level, so this level circled form makes no contribution to the circled forms of (m).

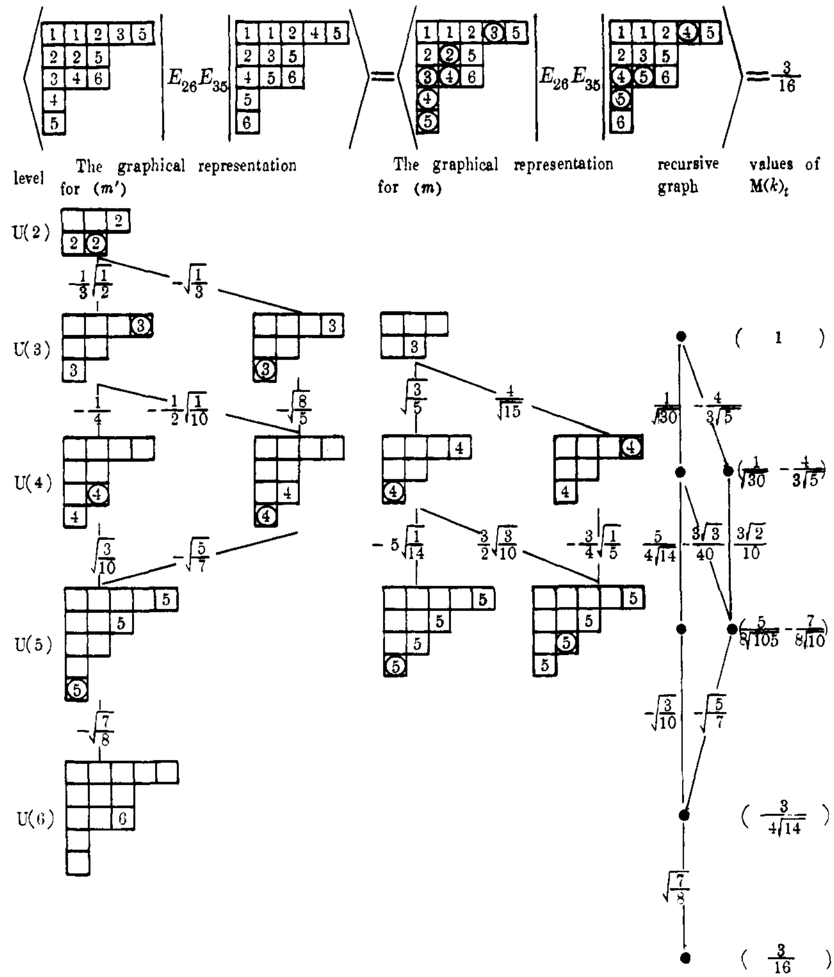


Figure 7. An example of the partially overlapping type, which is for the extension of $\langle (m')|E_{ji}E_{ji}|(m)\rangle$.

box, which is larger than k, must be contained in a circle. The recursive graph can be established from level i to level j, rather than from j to i, for the easy determination of which boxes the hidden circled k can be entered in. And the recursive evaluation is also carried out from level i to level j, with $M(i)_t = 1$ and $\langle (m')|E_{ij}E_{ji}|(m)\rangle = M(j)_1$. In figure 6, an example for this case is given.

3.4. *Partial overlapping*

Finally, we shall discuss the partially overlapping type only briefly. The circled numbers can be divided into two sets. The first set are in the non-overlapping range and can be determined definitely by means of comparison. The second set, however, are in the overlapping range, and the procedures obtained above for the cases in subsections 3.1–3.3 are needed to define their positions. One can see, furthermore, from the factorisation of one-body operator matrix elements i.e. equations (2) and (3), that the formulae for multistep operators $E_{i,i-k}$ are similar to those for one-step operators $E_{i,i-1}$. The extra factor H is, unlike the work of Kent and Schlesinger, independent of the shapes of linkages. Therefore, the treatment of the partially overlapping type may be just taken to be the extension of the three fully overlapping cases according to whether E_1 and E_2^+ are raising or lowering operators. The procedures of evaluation would become similar. Here we only show two examples as in figures 7 and 8.

4. Discussion

The study of the two-body operator matrix elements for many-particle systems is a complex one. The recursive scheme presented in this paper implies a factorisation scheme where each level produces a factor which can be separately evaluated. To obtain the complete matrix element one compiles all the separate factors. The key problem remaining is how to contain the information pertinent to the description of very large bases within computer memory. This is what we shall focus on in future work.

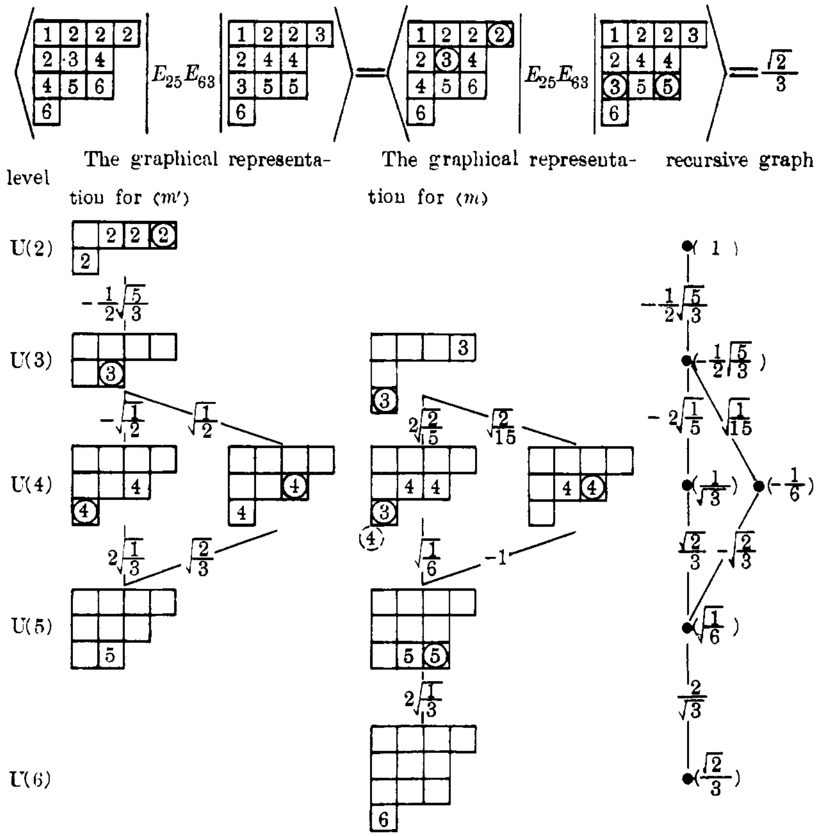


Figure 8. An example of the partially overlapping type, which is for the extension of $\langle (m')|E_{ji}E_{ij}|(m)\rangle$.

Acknowledgment

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