

Got Tensor Contractions?

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July 25, 2020

1 DEFINITIONS

1. The values of consecutive indices which are not separated by commas are assumed to form an ascending sequence (partially symmetrical storage).
2. Index groups separated by commas run independently.
3. Index ranges:
m,n,l: full occupied orbital range (e.g., [0..99]);
e,f,d: full virtual orbital range (e.g., [100..999]);
I,J,K: a small (active) subrange of the occupied orbital range (e.g., [90..99]);
A,B,C: a small (active) subrange of the virtual orbital range (e.g., [990..999]);
i,j,k: the occupied orbital range excluding the active subrange (e.g., [0..89]);
a,b,c: the virtual orbital range excluding the active subrange (e.g., [100..989]).
4. Despite multiple forms in which S/L/C tensors may appear in contractions, the only unique elements of these tensors are those which have both upper and lower indices ordered in an ascending order (separately).

2 TENSOR EXPRESSIONS

- (1) $3 : Z+ = H_{d_1}^{l_1} S_{l_1}^{d_1}$
- (2) $9 : Z+ = H_{d_1 d_2}^{l_1 l_2} S_{l_1 l_2}^{d_1 d_2}$
- (3) $18 : Z+ = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{d_1} S_{l_2}^{d_2} \cdot 1/2$
- (4) $1 : Z_{m_1}^{e_1} + = H_{m_1}^{e_1}$
- (5) $4 : Z_{m_1}^{e_1} + = H_{d_1}^{e_1} S_{m_1}^{d_1}$
- (6) $5 : Z_{m_1}^{e_1} + = H_{m_1}^{l_1} S_{l_1}^{e_1} \cdot -1/1$
- (7) $6 : Z_{m_1}^{e_1} + = H_{m_1, d_1}^{e_1, l_1} S_{l_1}^{d_1}$
- (8) $10 : Z_{m_1}^{e_1} + = H_{d_1}^{l_1} S_{m_1, l_1}^{e_1, d_1}$
- (9) $11 : Z_{m_1}^{e_1} + = H_{d_1 d_2}^{e_1, l_1} S_{m_1, l_1}^{d_1 d_2}$
- (10) $12 : Z_{m_1}^{e_1} + = H_{m_1, d_1}^{l_1 l_2} S_{l_1 l_2}^{e_1, d_1} \cdot -1/1$
- (11) $19 : Z_{m_1}^{e_1} + = H_{d_1}^{l_1} S_{l_1}^{e_1} S_{m_1}^{d_1} \cdot -1/1$
- (12) $20 : Z_{m_1}^{e_1} + = H_{d_1, d_2}^{e_1, l_1} S_{m_1}^{d_1} S_{l_1}^{d_2}$
- (13) $21 : Z_{m_1}^{e_1} + = H_{m_1, d_1}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{d_1} \cdot -1/1$
- (14) $25 : Z_{m_1}^{e_1} + = H_{d_1 d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{m_1, l_2}^{d_1 d_2} \cdot -1/1$

- (15) $26 : Z_{m_1}^{e_1} + = H_{d_1, d_2}^{l_1 l_2} S_{m_1}^{d_1} S_{l_1 l_2}^{e_1, d_2} \cdot -1/1$
- (16) $27 : Z_{m_1}^{e_1} + = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{d_1} S_{m_1, l_2}^{e_1, d_2}$
- (17) $40 : Z_{m_1}^{e_1} + = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{m_1}^{d_1} S_{l_2}^{d_2} \cdot -1/1$
- (18) $2 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1 m_2}^{e_1 e_2}$
- (19) $7 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{e_1 e_2} S_{m_2}^{d_1}$
- (20) $8 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1 m_2}^{e_1, l_1} S_{l_1}^{e_2} \cdot -1/1$
- (21) $13 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1}^{e_1} S_{m_1 m_2}^{e_2, d_1} \cdot -1/1$
- (22) $14 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1}^{l_1} S_{m_2, l_1}^{e_1 e_2}$
- (23) $15 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1 d_2}^{e_1 e_2} S_{m_1 m_2}^{d_1 d_2}$
- (24) $16 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{e_1, l_1} S_{m_2, l_1}^{e_2, d_1}$
- (25) $17 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1 m_2}^{l_1 l_2} S_{l_1 l_2}^{e_1 e_2}$
- (26) $22 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{e_1 e_2} S_{m_1}^{d_1} S_{m_2}^{d_2} \cdot 1/2$
- (27) $23 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{e_1, l_1} S_{l_1}^{e_2} S_{m_2}^{d_1} \cdot -1/1$
- (28) $24 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1 m_2}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{e_2} \cdot 1/2$
- (29) $28 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1}^{l_1} S_{l_1}^{e_1} S_{m_1 m_2}^{e_2, d_1}$
- (30) $29 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1}^{l_1} S_{m_1}^{d_1} S_{m_2, l_1}^{e_1 e_2}$
- (31) $30 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1 d_2}^{e_1, l_1} S_{l_1}^{e_2} S_{m_1 m_2}^{d_1 d_2} \cdot -1/1$
- (32) $31 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{e_1, l_1} S_{m_1}^{d_1} S_{m_2, l_1}^{e_2, d_2}$
- (33) $32 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{e_1, l_1} S_{l_1}^{d_1} S_{m_1 m_2}^{e_2, d_2}$
- (34) $33 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{l_1, l_2} S_{l_1}^{e_1} S_{m_2, l_2}^{e_2, d_1} \cdot -1/1$
- (35) $34 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{l_1 l_2} S_{m_2}^{d_1} S_{l_1 l_2}^{e_1 e_2}$
- (36) $35 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{l_1, l_2} S_{l_1}^{d_1} S_{m_2, l_2}^{e_1 e_2} \cdot -1/1$
- (37) $36 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1 d_2}^{l_1, l_2} S_{m_1, l_1}^{e_1 e_2} S_{m_2, l_2}^{d_1 d_2} \cdot -1/1$
- (38) $37 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1 d_2}^{l_1 l_2} S_{l_1 l_2}^{e_1 e_2} S_{m_1 m_2}^{d_1 d_2}$
- (39) $38 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1 l_2} S_{m_1 m_2}^{e_1, d_1} S_{l_1 l_2}^{e_2, d_2} \cdot -1/1$
- (40) $39 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1, l_2} S_{m_1, l_1}^{e_1, d_1} S_{m_2, l_2}^{e_2, d_2} \cdot 1/2$
- (41) $41 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{e_1, l_1} S_{l_1}^{e_2} S_{m_1}^{d_1} S_{m_2}^{d_2} \cdot -1/2$
- (42) $42 : Z_{m_1 m_2}^{e_1 e_2} + = H_{m_1, d_1}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{e_2} S_{m_2}^{d_1} \cdot 1/2$
- (43) $43 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1 d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{e_2} S_{m_1 m_2}^{d_1 d_2} \cdot 1/2$
- (44) $44 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{m_1}^{d_1} S_{m_2, l_2}^{e_2, d_2} \cdot -1/1$
- (45) $45 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{d_1} S_{m_1 m_2}^{e_2, d_2} \cdot -1/1$
- (46) $46 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1 l_2} S_{m_1}^{d_1} S_{m_2}^{d_2} S_{l_1 l_2}^{e_1 e_2} \cdot 1/2$
- (47) $47 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1, l_2} S_{m_1}^{d_1} S_{l_1}^{d_2} S_{m_2, l_2}^{e_1 e_2} \cdot -1/1$
- (48) $48 : Z_{m_1 m_2}^{e_1 e_2} + = H_{d_1, d_2}^{l_1, l_2} S_{l_1}^{e_1} S_{l_2}^{e_2} S_{m_1}^{d_1} S_{m_2}^{d_2} \cdot 1/4$