S^2 SAJÁTFÜGGVÉNYEINEK SZERKESZTÉSE SPINOPERÁTOROS MÓDSZERREL

doktori értekezés

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Tartalom

1. § Bevezetés

Mivel a hullámegyenlet egzakt megoldása csak néhány, meglehetősen speciális alakban felvett potenciálfüggvény esetében lehetséges, kvantumkémiai problémák megoldásánál közelitő eljárásokra vagyunk utalva.

Ezek közül a század közepén a konfigurációs kölcsönhatás módszere került előtérbe. Ennél a módszernél a nulladrendü sajátfüggvényt SLATER-determinánsok lineáris kombinációjaként adjuk meg. Az energiát pedig a szokásos szekuláris egyenlet gyökei szolgáltatják. Minthogy nincs utasitásunk arra vonatkozólag, hogy a SLATER-determinánsokkal megadott konfigurációk közül melyek a fontosak és melyek az elhanyagolhatóak, a szekuláris egyenlet redukálására új módszerek kidolgozása vált szükségessé, melyek közül egyik lehet a spinoperátoros eljárás.

2. § Spinoperátorok

A spektrumok multiplett szerkezetének és az anomális ZEEMANN-effektusnak elméleti alátámasztása céljából GOUDSMIT és UHLENBECK feltették, hogy az elektron, a keringésével együttjáró pálya-impulzusmomentum mellett, egy saját-impulzusmomentummal is rendelkezik. Ezt spinnek nevezték.

Kvantummechanikából ismeretes az $\mathbb{L}$ impulzusmomentum operátor sajátértékegyenlete:

$$\mathbb{L}\psi = \hbar\sqrt{l(l+1)}\,\psi. \qquad / 2.1 /$$

Tehát az előbbiek alapján / 2.1 / a spinoperátorra is érvényes:

$$\mathbb{S}\psi = \hbar\sqrt{s(s+1)}\,\psi. \qquad / 2.2 /$$

Az impulzusmomentum operátor felcserélési relációja alapján :

$$\begin{aligned} \mathbb{S}_x\mathbb{S}_y - \mathbb{S}_y\mathbb{S}_x &= i\hbar\,\mathbb{S}_z \\ \mathbb{S}_y\mathbb{S}_z - \mathbb{S}_z\mathbb{S}_y &= i\hbar\,\mathbb{S}_x \\ \mathbb{S}_z\mathbb{S}_x - \mathbb{S}_x\mathbb{S}_z &= i\hbar\,\mathbb{S}_y . \end{aligned} \qquad / 2.3 /$$

A spinoperátorok mátrixelőállításai a következők:

$$\begin{aligned} \mathbb{S}_x &= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \mathbb{S}_y &= \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \mathbb{S}_z &= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \end{aligned} \qquad / 2.4 /$$

Az itt szereplő mátrixok az u.n. PAULI-féle spinmátrixok.

A spin kvantálása pedig a következő egyenletek alapján történik :

$$\mathfrak{S}^2 = \hbar\, l_s(l_s+1), \quad \text{ahol} \quad l_s = \frac{1}{2}$$

$$\mathfrak{S}_z = \hbar\, m_s \quad , \quad \text{ahol} \quad m_s = \pm\frac{1}{2}, \qquad / 2.5 /$$

m_s a spinkvantumszám. Az $m_s = +\frac{1}{2}$ -hez tartozó egyrészecske spinfüggvényt α -val, az $m_s = -\frac{1}{2}$ -hez tartozó egyrészecske spinfüggvényt β -val jelöljük. Ezek mátrixokkal a következőképpen állithatók elő :

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \qquad / 2.6 /$$

/ 2.4 / és / 2.6 / alapján belátható a következő egyenletek érvényessége :

$$\begin{aligned} \mathfrak{S}_x \alpha &= \frac{\hbar}{2}\beta \\ \mathfrak{S}_y \alpha &= \frac{\hbar}{2} i\beta \\ \mathfrak{S}_z \alpha &= \frac{\hbar}{2}\alpha , \end{aligned} \qquad / 2.7 /$$

$$\begin{aligned} \mathfrak{S}_x \beta &= \frac{\hbar}{2}\alpha \\ \mathfrak{S}_y \beta &= -\frac{\hbar}{2} i\alpha \\ \mathfrak{S}_z \beta &= -\frac{\hbar}{2}\beta . \end{aligned} \qquad / 2.8 /$$

Vezessük be a következő spinoperátorokat :

$$\mathfrak{S}^+ = \mathfrak{S}_x + i\,\mathfrak{S}_y \qquad / 2.9 /$$

$$\mathfrak{S}^- = \mathfrak{S}_x - i\,\mathfrak{S}_y . \qquad / 2.10 /$$

Előbbiek alapján :

$$\begin{aligned} \mathfrak{S}^+\alpha &= 0 \qquad & \mathfrak{S}^+\beta &= \hbar\alpha \\ \mathfrak{S}^-\alpha &= \hbar\beta \qquad & \mathfrak{S}^-\beta &= 0 . \end{aligned} \qquad / 2.11 /$$

/ 2.11 / egyenletek miatt $\mathfrak{S}^+$-t felfelé, - $\mathfrak{S}^-$-t pedig lefelé forditó spinoperátoroknak nevezzük. Az $\mathfrak{S}^2$ operátornak a fel és lefelé forditó spinoperátorokkal való összefüggését / 2.7 /, / 2.8 /, / 2.11 / alapján a következő egyenlet adja :

$$\mathfrak{S}^2 = (\mathfrak{S}_x + i\mathfrak{S}_y)(\mathfrak{S}_x - i\mathfrak{S}_y) + \mathfrak{S}_z^2 - i(\mathfrak{S}_x\mathfrak{S}_y - \mathfrak{S}_y\mathfrak{S}_x),$$

$$\mathfrak{S}^2 = \mathfrak{S}^+\mathfrak{S}^- + \mathfrak{S}_z^2 - \hbar\mathfrak{S}_z . \qquad / 2.12 /$$

Hasonlóan adódik a következő összefüggés is :

$$\mathfrak{S}^2 = \mathfrak{S}^-\mathfrak{S}^+ + \mathfrak{S}_z^2 + \hbar\mathfrak{S}_z . \qquad / 2.13 /$$

Több elektron esetén a rendszerre vonatkozó fel,- és lefelé forditó spinoperátor és az $\mathfrak{S}_z$ operátor a következő alaku :

$$\mathfrak{S}^+ = \sum_{i=1}^{n} \mathfrak{S}_i^+ , \quad \mathfrak{S}^- = \sum_{i=1}^{n} \mathfrak{S}_i^- , \quad \mathfrak{S}_z = \sum_{i=1}^{n} \mathfrak{S}_{iz} \qquad / 2.14 /$$

ahol n az elektronok számát jelenti.

3. § Összefüggések az S_z operátor sajátfüggvényei között

A következőkben $\hbar$ egységekben dolgozunk. Legyen adott egy s eredő spinű rendszer, amelynek állapotát $\psi(s, m_s)$ sajátfüggvény irja le. A z tengelyre vonatkozó spinvetületek a következők :

$$m_s = s, \dots, s-i, \dots -s. \qquad / 3.1 /$$

A megfelelő sajátfüggvények pedig :

$$\psi(s,s), \dots, \psi(s,s-i), \dots, \psi(s,-s). \qquad / 3.2 /$$

Ezeket rendre maximális, i-edik és minimális komponenseknek nevezzük.

VAN DER WAERDEN [4] alapján ismeretes, hogy a fel- és lefelé forditó spinoperátorok hatására bármelyik komponensből az utána következő, ill. az előtte álló komponenssel arányos sajátfüggvényt nyerjük a következő összefüggések alapján :

$$\begin{aligned} S^+ \psi(s,\mu) &= [(s-\mu)(s+\mu+1)]^{\frac{1}{2}} \psi(s,\mu+1) \\ S^- \psi(s,\mu) &= [(s+\mu)(s-\mu+1)]^{\frac{1}{2}} \psi(s,\mu-1). \end{aligned} \qquad / 3.3 /$$

Bármelyik komponens kifejezhető a maximális, ill. minimális komponensből / 3.3 / alapján :

$$\psi(s, s-i) = \frac{1}{i!} \binom{2s}{i}^{-\frac{1}{2}} (S^-)^i \psi(s,s) \qquad / 3.4 /$$

$$\psi(s, s+i) = \frac{1}{i!} \binom{2s}{i}^{-\frac{1}{2}} (S^+)^i \psi(s,-s). \qquad / 3.5 /$$

4. § A spinösszetevés operátora

Legyen adott két rendszer : A_1 és A_2 melyeknek eredő spinjei s és s' . A megfelelő sajátfüggvények : $\psi_{A_1}(s,m_s)$ és $\psi_{A_2}(s',m_{s'})$. Ezek az $\mathfrak{S}_z$ operátor sajátfüggvényei, azaz :

$$\mathfrak{S}_z\, \psi_{A_1}(s,m_s) = m_s\, \psi_{A_1}(s,m_s)$$
$$\mathfrak{S}_z\, \psi_{A_2}(s',m_{s'}) = m_{s'}\, \psi_{A_2}(s',m_{s'}). \qquad /\ 4.1\ /$$

Egyesitsük a két rendszert. Az egyesitett rendszer állapotát leiró sajátfüggvények közül a maximális komponens VAN DER WAERDEN [4] szerint a következő alakú :

$$\Psi(S,M_S) = \binom{2s+2s'-\lambda+1}{\lambda}^{-\frac{1}{2}} \sum_{i=0}^{\lambda} (-1)^i \left[\binom{2s-i}{\lambda-i}\binom{2s'+i-\lambda}{i}\right]^{\frac{1}{2}} \times$$
$$\times\, \psi_{A_1}(s,s-i)\, \psi_{A_2}(s',s'+i-\lambda). \qquad /\ 4.2\ /$$

Két fontos speciális esetet vizsgálunk :

1./ $\lambda=0$ ekkor $S=s+s'$ és

$$\Psi(S=s+s',M_S=s+s') = \psi_{A_1}(s,s)\, \psi_{A_2}(s',-s'+i), \qquad /4.3\ /$$

azaz az s spinü rendszerhez hozzáadtunk egy s' spinü rendszert, és egy $s+s'$ spinü rendszert nyertünk.

2./ $\lambda=2s'$ ekkor $S=s-s'$ és

$$\Psi(S=s-s',M_s=s-s') = \binom{2s+1}{2s'}^{-\frac{1}{2}} \sum_{i=0}^{2s'} (-1)^i \binom{2s-i}{2s'-i}^{\frac{1}{2}} \psi_{A_1}(s,s-i)\, \psi_{A_2}(s',-s'+i), \qquad /\ 4.4\ /$$

azaz az s spinü rendszerből kivontuk az s' spinü rendszert és egy $s-s'$ spinü rendszert nyertünk. A / 4.3 / és / 4.4 / egyenletek a spinösszeadás és spinkivonás egyenletei.

BERENCZ F. [1] bebizonyitotta, hogy a VAN DER WAERDEN-féle / 4.2 / alatti spinösszetevési egyenlet $\mathfrak{S}^2$ sajátfüggvényét adja $(s+s'-\lambda)(s+s'-\lambda+1)$ sajátértékkel.

Irjuk át a spinösszetevés egyenletét / 3.4 / alapján a spinoperátorokkal :

$$\Psi(S,M_S) = \binom{2s+2s'-\lambda+1}{\lambda}^{-\frac{1}{2}} \sum_{i=0}^{\lambda} (-1)^i \left[\binom{2s-i}{\lambda-i}\binom{2s'+i-\lambda}{i}\right]^{\frac{1}{2}} \times$$

$$\times \frac{1}{i!}\binom{2s}{i}^{-\frac{1}{2}} \frac{1}{(\lambda-i)!}\binom{2s'}{\lambda-i}^{-\frac{1}{2}} (\mathfrak{S}^-_{A_1})^i (\mathfrak{S}^-_{A_2})^{\lambda-i} \psi_{A_1}(s,s)\,\psi_{A_2}(s',s')$$

$$\Psi(S,M_S) = \binom{2s+2s'-\lambda+1}{\lambda}^{-\frac{1}{2}} [(2s)!(2s')!(2s-\lambda)!(2s'-\lambda)!]^{-\frac{1}{2}} \times$$

$$\times \sum_{i=0}^{\lambda} (-1)^i \frac{(2s-i)!(2s'+i-\lambda)!}{i!(\lambda-i)!} (\mathfrak{S}^-_{A_1})^i (\mathfrak{S}^-_{A_2})^{\lambda-i} \psi_{A_1}(s,s)\,\psi_{A_2}(s',s'). \qquad / 4.5 /$$

/ 4.5 / alapján tehát az operátor, amellyel $\mathfrak{S}^2$ sajátfüggvényeit nyerjük, a következő alakú :

$$\mathbb{O}(S=s+s'-\lambda, M_S=s+s'-\lambda) = \binom{2s+2s'-\lambda+1}{\lambda}^{-\frac{1}{2}} \times$$

$$\times [(2s)!(2s')!(2s-\lambda)!(2s'-\lambda)!]^{-\frac{1}{2}} \times \qquad / 4.6 /$$

$$\times \sum_{i=0}^{\lambda} (-1)^i \frac{(2s-i)!(2s'+i-\lambda)!}{i!\,(\lambda-i)!} (\mathfrak{S}^-_{A_1})^i (\mathfrak{S}^-_{A_2})^{\lambda-i}.$$

A / 3.5 / egyenletet felhasználva megadhatjuk operátorunknak azt az alternativ alakját, amelyben már az $\mathfrak{S}^+$ operátor is szerepel :

$$\Psi(S,M_S) = \left(\frac{2s-2s'+1}{2s+1}\right)^{\frac{1}{2}} \sum_{i=0}^{2s'} (-1)^i \frac{(2s-i)!}{(2s)!\,i!} \times$$

$$\times (\mathfrak{S}^-_{A_1} \mathfrak{S}^+_{A_2})^i \psi_{A_1}(s,s)\,\psi_{A_2}(s',-s'). \qquad / 4.7 /$$

A megfelelő operátor tehát a következő alaku :

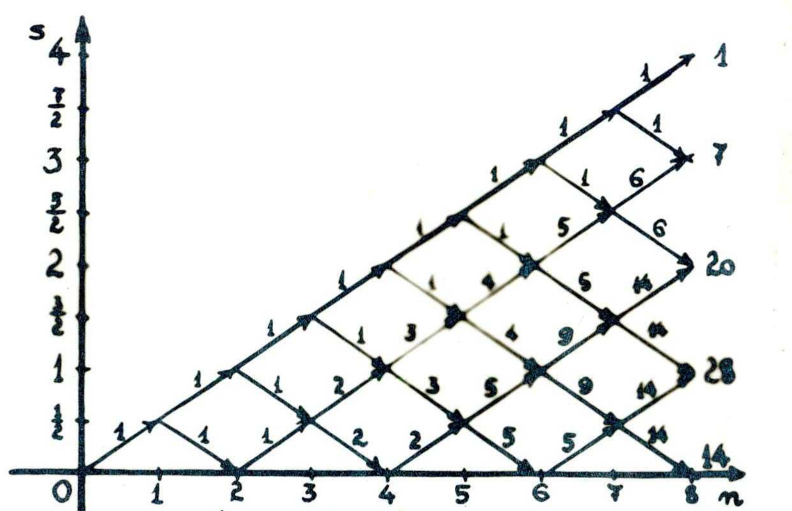
$$\mathbb{O}(S, M_S) = \left(\frac{2S - 2S' + 1}{2S + 1} \right)^{\frac{1}{2}} \times \sum_{i=0}^{2S'} (-1)^i \frac{(2S-i)!}{(2S)!\, i!} \left(\mathbb{S}_{A_1}^- \mathbb{S}_{A_2}^+ \right)^i . \qquad / 4.8 /$$

5. § A spinösszetevés operátora SLATER- determinánsokkal megadott sajátfüggvények esetében

Egy n elektronból álló rendszer lineárisan független spinállapotainak a számát s eredő spin esetén CORSON [2] szerint a következőképpen számithatjuk ki :

$$N(s) = \binom{n}{\frac{n}{2}-s} - \binom{n}{\frac{n}{2}-s-1} \qquad /\ 5.1\ /$$

Ezt a számot az elágazási diagramból is leolvashatjuk :



ELÁGAZÁSI DIAGRAM

/ A diagramban feltüntetett számok a vonalak multiplicitását jelentik. / Az elágazási diagram a spinállapotok szerkesztési módját mutatja. Eszerint egy n elektronból álló rendszer S eredő spinü állapota olymódon konstruálható meg, hogy x_1 számu, párhuzamos α spinü elektronból álló rendszerhez hozzáadunk x_2 számu, párhuzamos β

spinű elektronból álló rendszert; majd az egyesitett rendszerhez hozzáadjuk az x_3 számu α spinű elektronból álló rendszert stb. Ezt az eljárást addig folytatjuk, mig az összes elektront figyelembe nem vettük. Ha a részrendszerek állapotát SLATER- determinánsokkal irtuk le, akkor / 4.6 / és / 4.8 / alkalmazásával $\mathfrak{S}^2$ sajátfüggvényeit kapjuk.

A továbbiakban / 4.6 / és / 4.8 / egyenleteknek SLATER- determinánsokra vonatkozó alakját adjuk meg, majd alkalmazásként nyolc elektronból álló rendszer különböző multiplicitásu spinállapotait számitjuk ki. Ezt azért tehetjük, mert BERENCZ F. [1] bebizonyitotta, hogy / 3.3 / egyenletek speciálisan SLATER- determináns alakban felvett sajátfüggvényekre is érvényesek.

A SLATER- determinánsokat a következőképpen jelöljük:

$$\varphi(S, m_S) = |\alpha\alpha\beta\ldots\alpha| . \qquad / 5.2 /$$

Legyen x_1 elektronunk párhuzamos α spinnel. Egyesitsük ezeket $S=\frac{x_1}{2}$ eredő spinű rendszerré / A_1 /, az A_1 rendszer maximális komponense / 4.3 / szerint

$$\varphi_{A_1}\left(S = \frac{x_1}{2}, m_S = \frac{x_1}{2}\right) = |\overset{1,}{\alpha}\overset{2,\ldots,}{\alpha}\ldots\overset{x_1}{\alpha}| . \qquad / 5.3 /$$

Legyen x_2 elektronunk párhuzamos β spinnel. Egyesitsük ezeket $S'=\frac{x_2}{2}$ eredő spinű rendszerré / A_2 /, az A_2 rendszer minimális komponense :

$$\varphi_{A_2}\left(S' = \frac{x_2}{2}, m_{S'} = -\frac{x_2}{2}\right) = |\overset{1,}{\beta}\overset{2,}{\beta}\ldots\overset{x_2}{\beta}| . \qquad / 5.4 /$$

Egyesitsük az A_1 és A_2 rendszert $S-S' = \frac{x_1}{2} - \frac{x_2}{2}$ eredő spinnel, akkor / 4.7 / szerint az egyesitett rendszer maximális komponense a következő alaku :

$$\varphi_{A_1A_2}(S,m_S)=\left(\frac{x_1-x_2+1}{x_1-1}\right)^{\frac{1}{2}}\sum_{i=0}^{x_2}(-1)^i\frac{(x_1-i)!}{x_1!\,i!}\left(\mathfrak{S}_{A_1}^-\mathfrak{S}_{A_2}^+\right)^i|\overset{1,\dots,x_1}{\alpha\dots\alpha}\overset{1,\dots,x_2}{\beta\dots\beta}|. \qquad /\ 5.5\ /$$

A megfelelő operátor tehát :

$$\mathbb{O}_{A_1A_2}=\left(\frac{x_1-x_2+1}{x_1+1}\right)^{\frac{1}{2}}\sum_{i=0}^{x_2}(-1)^i\frac{(x_1-i)!}{x_1!\,i!}\left(\mathfrak{S}_{A_1}^-\mathfrak{S}_{A_2}^+\right)^i. \qquad /\ 5.6\ /$$

Az A_1A_2 rendszerhez adjuk hozzá az A_3 rendszert olymódon, hogy az eredő spin $\frac{x_1-x_2+x_3}{2}$ legyen. Ekkor

$$\varphi_{A_1A_2A_3}=\mathbb{O}_{A_1A_2}|\overset{1,\dots,x_1}{\alpha\dots\alpha}\overset{1,\dots,x_2}{\beta\dots\beta}\overset{1,\dots,x_3}{\alpha\dots\alpha}|. \qquad /\ 5.7\ /$$

Adjunk hozzá $A_1A_2A_3$ rendszerhez A_4 rendszert olymódon, hogy az eredő spin $\frac{x_1-x_2+x_3-x_4}{2}$ legyen. Az egyesitett rendszer maximális komponense :

$$\varphi_{A_1A_2A_3A_4}=\left(\frac{x_1-x_2+x_3-x_4+1}{x_1-x_2+x_3+1}\right)^{\frac{1}{2}}\left(\frac{x_1-x_2+1}{x_1+1}\right)^{\frac{1}{2}}\sum_{i=0}^{x_4}(-1)^i\times$$

$$\times\frac{(x_1-x_2+x_3-i)!}{(x_1+x_2+x_3)!\,i!}\left(\mathfrak{S}_{A_1A_2A_3}^-\mathfrak{S}_{A_4}^+\right)^i\sum_{j=0}^{x_2}(-1)^j\frac{(x_1-j)!}{x_1!\,j!}\times \qquad /\ 5.8\ /$$

$$\times\left(\mathfrak{S}_{A_1}^-\mathfrak{S}_{A_2}^+\right)^j|\overset{1,\dots,x_1}{\alpha\dots\alpha}\overset{1,\dots,x_2}{\beta\dots\beta}\overset{1,\dots,x_3}{\alpha\dots\alpha}\overset{1,\dots,x_4}{\beta\dots\beta}|.$$

A megfelelő operátor :

$$\mathbb{O}_{A_1A_2A_3A_4}=\left(\frac{x_1-x_2+x_3-x_4+1}{x_1-x_2+x_3+1}\right)^{\frac{1}{2}}\left(\frac{x_1-x_2+1}{x_1+1}\right)^{\frac{1}{2}}\sum_{i=0}^{x_4}(-1)^i\times$$

$$\times\frac{(x_1-x_2+x_3-i)!}{(x_1-x_2+x_3)!\,i!}\left(\mathfrak{S}_{A_1A_2A_3}^-\mathfrak{S}_{A_4}^+\right)^i\sum_{j=0}^{x_2}(-1)^j\frac{(x_1-j)!}{x_1!\,j!}\left(\mathfrak{S}_{A_1}^-\mathfrak{S}_{A_2}^+\right)^j. \qquad /\ 5.9\ /$$

Az előbb látott módon adjunk hozzá az $A_1A_2A_3A_4$ rendszerhez további A_5 , A_6 ,... stb. rendszereket, amig valamennyi elektront figyelembe nem vettünk.

Akkor pl. nyolc rendszer egyesitése esetén a következő operátort nyerjük :

$$\mathbb{O}_{A_1A_2A_3A_4A_5A_6A_7A_8} = \left(\frac{x_1-x_2+x_3-x_4+x_5-x_6+x_7-x_8+1}{x_1-x_2+x_3-x_4+x_5-x_6+x_7+1}\right)^{\frac{1}{2}} \times$$

$$\times\left(\frac{x_1-x_2+x_3-x_4+x_5-x_6+1}{x_1-x_2+x_3-x_4+x_5+1}\right)^{\frac{1}{2}}\left(\frac{x_1-x_2+x_3-x_4+1}{x_1-x_2+x_3+1}\right)^{\frac{1}{2}}\left(\frac{x_1-x_2+1}{x_1+1}\right)^{\frac{1}{2}}\times$$

$$\times\sum_{i=0}^{x_8}(-1)^i\frac{(x_1-x_2+x_3-x_4+x_5-x_6+x_7-i)!}{(x_1-x_2+x_3-x_4+x_5-x_6+x_7)!\,i!}\left(\mathfrak{S}^-_{A_1A_2A_3A_4A_5A_6A_7}\mathfrak{S}^+_{A_8}\right)^i\times$$

$$\times\sum_{j=0}^{x_6}(-1)^j\frac{(x_1-x_2+x_3-x_4+x_5-j)!}{(x_1-x_2+x_3-x_4+x_5)!\,j!}\left(\mathfrak{S}^-_{A_1A_2A_3A_4A_5}\mathfrak{S}^+_{A_6}\right)^j\times \qquad /\ 5.1o\ /$$

$$\times\sum_{k=0}^{x_4}(-1)^k\frac{(x_1-x_2+x_3-k)!}{(x_1-x_2+x_3)!\,k!}\left(\mathfrak{S}^-_{A_1A_2A_3}\mathfrak{S}^+_{A_4}\right)^k\times$$

$$\times\sum_{l=0}^{x_2}(-1)^l\frac{(x_1-l)!}{x_1!\,l!}\left(\mathfrak{S}^-_{A_1}\mathfrak{S}^+_{A_2}\right)^l.$$

6. § Nyolc elektronos multiplettek

Ismeretes, hogy egy spinállapot multiplicitását a $2s+1$ szám adja meg, ahol s a spineredőt jelenti. A következő spinállapotok lehetségesek :

s	2s+1	A SPINÁLLAPOT NEVE
0	1	SZINGULETT
$\frac{1}{2}$	2	DOUBLETT
1	3	TRIPLETT
$\frac{3}{2}$	4	QUARTETT
2	5	QUINTETT
$\frac{5}{2}$	6	SZEXTETT
3	7	SZEPTETT
$\frac{7}{2}$	8	OKTETT
4	9	NONETT

Nyolc elektronból álló rendszer esetén a SLATER-determinánsok száma $2^8 = 256$. Ennek megfelelően az elágazási diagram szerint megszerkeszthetünk 14 szingulett, 28 triplett, 2o quintett, 7 szeptett és 1 nonett spinállapotot. / $14 \cdot 1 + 28 \cdot 3 + 20 \cdot 5 + 7 \cdot 7 + 1 \cdot 9 = 256$ / A továbbiakban a különböző multiplicitásu spinállapotok sajátfüggvényeit adjuk meg.

A./ Szingulettek

A 0 eredő spinhez tartozó SLATER- determinánsokat a következőképpen jelöljük :

$\varphi_1^0 = |\alpha\alpha\alpha\alpha\beta\beta\beta\beta|$

$\varphi_2^0 = |\alpha\alpha\alpha\beta\alpha\beta\beta\beta|$

$\varphi_3^0 = |\alpha\alpha\alpha\beta\beta\alpha\beta\beta|$

$\varphi_4^0 = |\alpha\alpha\alpha\beta\beta\beta\alpha\beta|$

$\varphi_5^0 = |\alpha\alpha\alpha\beta\beta\beta\beta\alpha|$

$\varphi_6^0 = |\alpha\alpha\beta\alpha\alpha\beta\beta\beta|$

$\varphi_7^0 = |\alpha\alpha\beta\alpha\beta\alpha\beta\beta|$

$\varphi_8^0 = |\alpha\alpha\beta\alpha\beta\beta\alpha\beta|$

$\varphi_9^0 = |\alpha\alpha\beta\alpha\beta\beta\beta\alpha|$

$\varphi_{10}^0 = |\alpha\alpha\beta\beta\alpha\alpha\beta\beta|$

$\varphi_{11}^0 = |\alpha\alpha\beta\beta\alpha\beta\alpha\beta|$

$\varphi_{12}^0 = |\alpha\alpha\beta\beta\alpha\beta\beta\alpha|$

$\varphi_{13}^0 = |\alpha\alpha\beta\beta\beta\alpha\alpha\beta|$

$\varphi_{14}^0 = |\alpha\alpha\beta\beta\beta\alpha\beta\alpha|$

$\varphi_{15}^0 = |\alpha\alpha\beta\beta\beta\beta\alpha\alpha|$

$\varphi_{16}^0 = |\alpha\beta\alpha\alpha\alpha\beta\beta\beta|$

$\varphi_{17}^0 = |\alpha\beta\alpha\alpha\beta\alpha\beta\beta|$

$\varphi_{18}^0 = |\alpha\beta\alpha\alpha\beta\beta\alpha\beta|$

$\varphi_{19}^0 = |\alpha\beta\alpha\alpha\beta\beta\beta\alpha|$

$\varphi_{20}^0 = |\alpha\beta\alpha\beta\alpha\alpha\beta\beta|$

$\varphi_{21}^0 = |\alpha\beta\alpha\beta\alpha\beta\alpha\beta|$

$\varphi_{22}^0 = |\alpha\beta\alpha\beta\alpha\beta\beta\alpha|$

$\varphi_{23}^0 = |\alpha\beta\alpha\beta\beta\alpha\alpha\beta|$

$\varphi_{24}^0 = |\alpha\beta\alpha\beta\beta\alpha\beta\alpha|$

$\varphi_{25}^0 = |\alpha\beta\alpha\beta\beta\beta\alpha\alpha|$

$\varphi_{26}^0 = |\alpha\beta\beta\alpha\alpha\alpha\beta\beta|$

$\varphi_{27}^0 = |\alpha\beta\beta\alpha\alpha\beta\alpha\beta|$

$\varphi_{28}^0 = |\alpha\beta\beta\alpha\alpha\beta\beta\alpha|$

$\varphi_{29}^0 = |\alpha\beta\beta\alpha\beta\alpha\alpha\beta|$

$\varphi_{30}^0 = |\alpha\beta\beta\alpha\beta\alpha\beta\alpha|$

$\varphi_{31}^0 = |\alpha\beta\beta\alpha\beta\beta\alpha\alpha|$

$\varphi_{32}^0 = |\alpha\beta\beta\beta\alpha\alpha\alpha\beta|$

$\varphi_{33}^0 = |\alpha\beta\beta\beta\alpha\alpha\beta\alpha|$

$\varphi_{34}^0 = |\alpha\beta\beta\beta\alpha\beta\alpha\alpha|$

$\varphi_{35}^0 = |\alpha\beta\beta\beta\beta\alpha\alpha\alpha|$

$\varphi_{36}^0 = |\beta\alpha\alpha\alpha\alpha\beta\beta\beta|$

$\varphi_{37}^0 = |\beta\alpha\alpha\alpha\beta\alpha\beta\beta|$

$\varphi_{38}^0 = |\beta\alpha\alpha\alpha\beta\beta\alpha\beta|$

$\varphi_{39}^0 = |\beta\alpha\alpha\alpha\beta\beta\beta\alpha|$

$\varphi_{40}^0 = |\beta\alpha\alpha\beta\alpha\alpha\beta\beta|$

$\varphi_{41}^0 = |\beta\alpha\alpha\beta\alpha\beta\alpha\beta|$

$\varphi_{42}^0 = |\beta\alpha\alpha\beta\alpha\beta\beta\alpha|$

$\varphi_{43}^0 = |\beta\alpha\alpha\beta\beta\alpha\alpha\beta|$

$\varphi_{44}^0 = |\beta\alpha\alpha\beta\beta\alpha\beta\alpha|$

$\varphi_{45}^0 = |\beta\alpha\alpha\beta\beta\beta\alpha\alpha|$

$\varphi_{46}^0 = |\beta\alpha\beta\alpha\alpha\alpha\beta\beta|$

$\varphi_{47}^0 = |\beta\alpha\beta\alpha\alpha\beta\alpha\beta|$

$\varphi_{48}^0 = |\beta\alpha\beta\alpha\alpha\beta\beta\alpha|$

$\varphi_{49}^0 = |\beta\alpha\beta\alpha\beta\alpha\alpha\beta|$

$\varphi_{50}^0 = |\beta\alpha\beta\alpha\beta\alpha\beta\alpha|$

$\varphi_{51}^0 = |\beta\alpha\beta\alpha\beta\beta\alpha\alpha|$

$\varphi_{52}^0 = |\beta\alpha\beta\beta\alpha\alpha\alpha\beta|$

$\varphi_{53}^0 = |\beta\alpha\beta\beta\alpha\alpha\beta\alpha|$

$\varphi_{54}^0 = |\beta\alpha\beta\beta\alpha\beta\alpha\alpha|$

$\varphi_{55}^0 = |\beta\alpha\beta\beta\beta\alpha\alpha\alpha|$

$\varphi_{56}^0 = |\beta\beta\alpha\alpha\alpha\alpha\beta\beta|$

$\varphi_{57}^0 = |\beta\beta\alpha\alpha\alpha\beta\alpha\beta|$

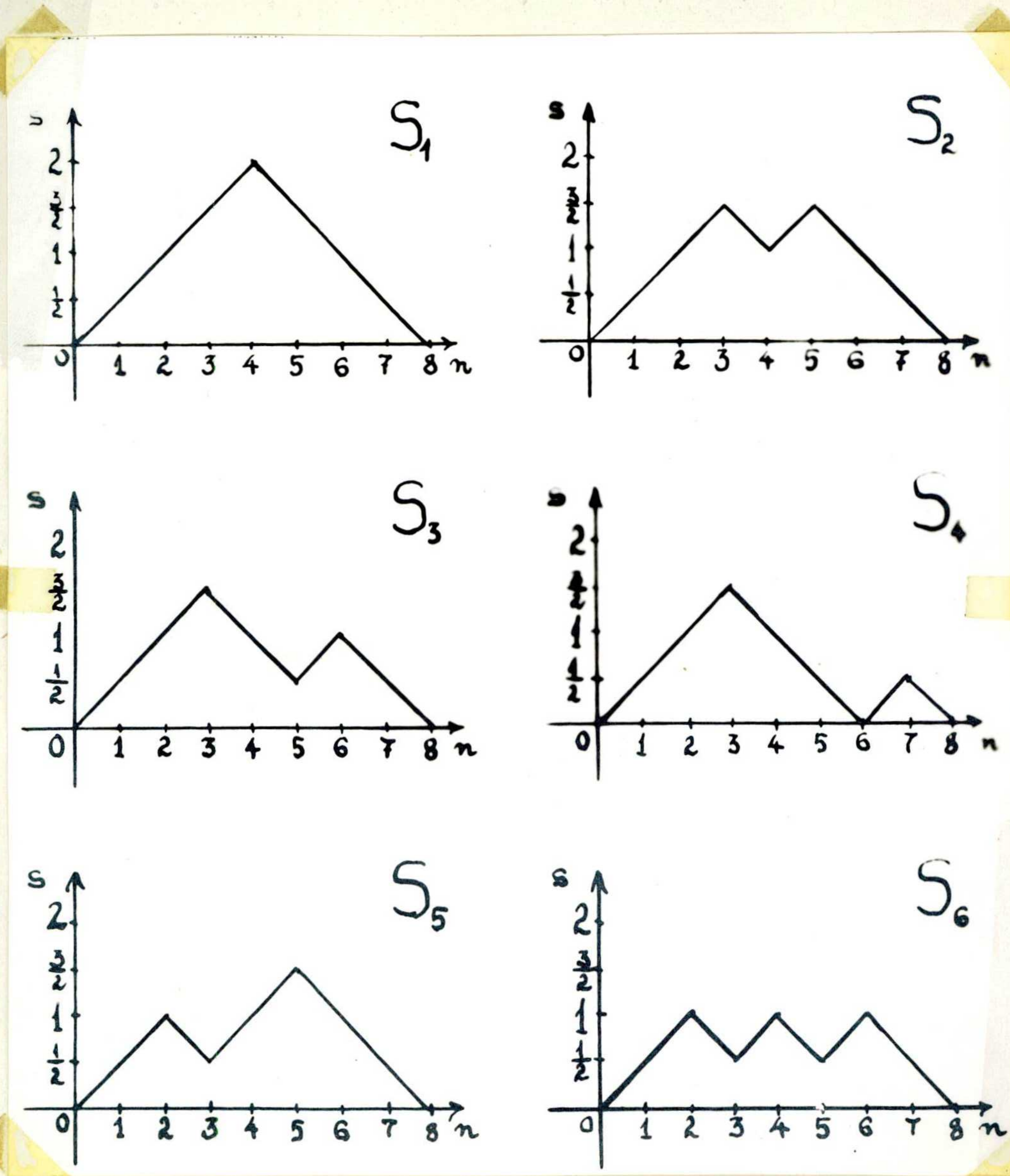
$\varphi_{58}^0 = |\beta\beta\alpha\alpha\alpha\beta\beta\alpha|$

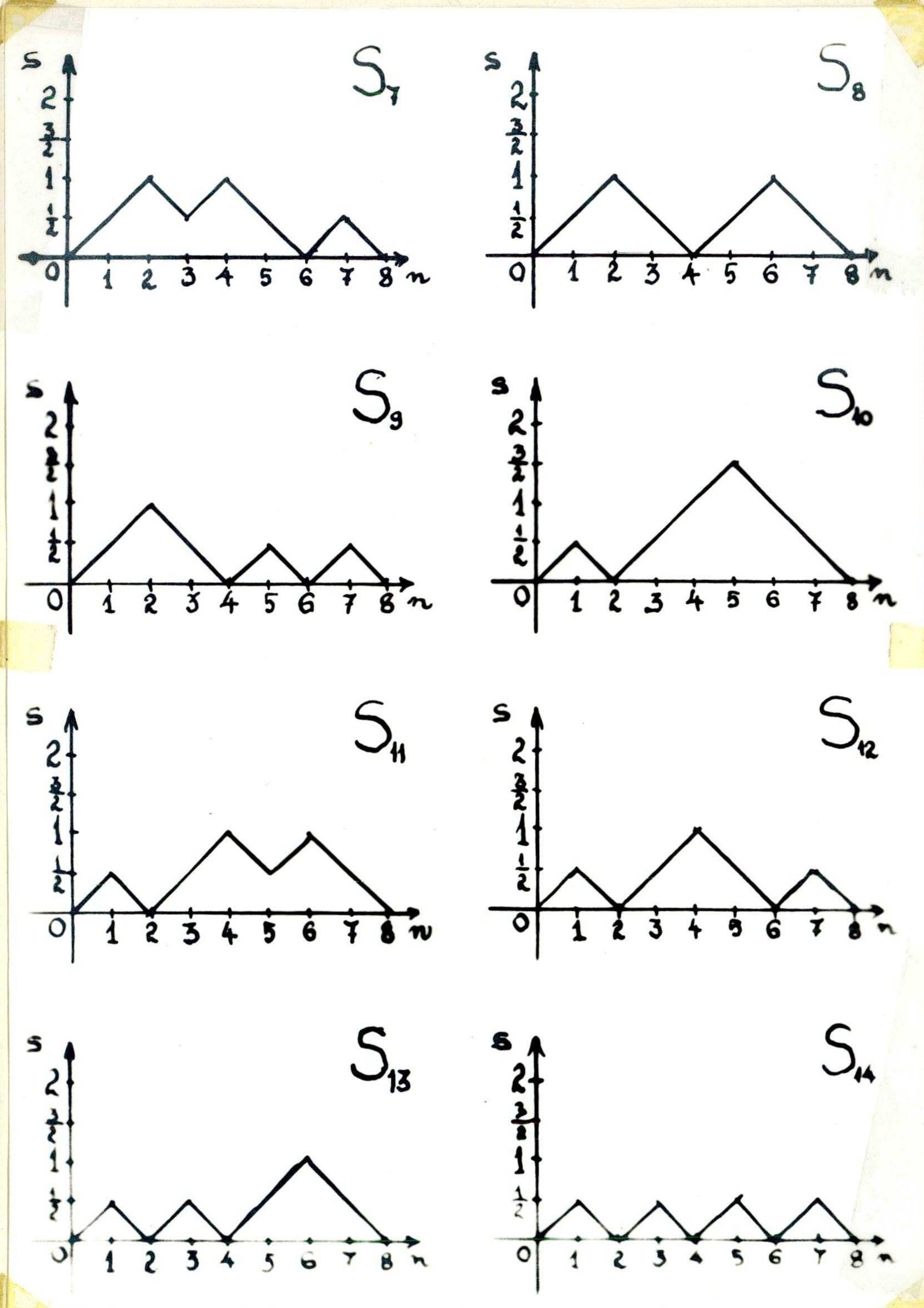
$\varphi_{59}^0 = |\beta\beta\alpha\alpha\beta\alpha\alpha\beta|$

$\varphi_{60}^0 = |\beta\beta\alpha\alpha\beta\alpha\beta\alpha|$

$$\varphi^{\circ}_{61} = |\beta\beta\alpha\alpha\beta\beta\alpha\alpha| \qquad \varphi^{\circ}_{66} = |\beta\beta\beta\alpha\alpha\alpha\alpha\beta|$$
$$\varphi^{\circ}_{62} = |\beta\beta\alpha\beta\alpha\alpha\alpha\beta| \qquad \varphi^{\circ}_{67} = |\beta\beta\beta\alpha\alpha\alpha\beta\alpha|$$
$$\varphi^{\circ}_{63} = |\beta\beta\alpha\beta\alpha\alpha\beta\alpha| \qquad \varphi^{\circ}_{68} = |\beta\beta\beta\alpha\alpha\beta\alpha\alpha|$$
$$\varphi^{\circ}_{64} = |\beta\beta\alpha\beta\alpha\beta\alpha\alpha| \qquad \varphi^{\circ}_{69} = |\beta\beta\beta\alpha\beta\alpha\alpha\alpha|$$
$$\varphi^{\circ}_{65} = |\beta\beta\alpha\beta\beta\alpha\alpha\alpha| \qquad \varphi^{\circ}_{70} = |\beta\beta\beta\beta\alpha\alpha\alpha\alpha|$$

Szinguletteket az elágazási diagram szerint 14 féleképpen szerkeszthetünk :




S7
S8
S9
S10
S11
S12
S13
S14

A megfelelő sajátfüggvények / 5.1o / alapján a következők:

$$
\begin{aligned}
\varphi_{S_1} = \frac{\sqrt{5}}{60}\{ & 12(\varphi_1^\circ + \varphi_{70}^\circ) + \\
& + 2(\varphi_{10}^\circ + \varphi_{11}^\circ + \varphi_{12}^\circ + \varphi_{13}^\circ + \varphi_{14}^\circ + \varphi_{15}^\circ + \varphi_{20}^\circ + \varphi_{21}^\circ + \varphi_{22}^\circ + \varphi_{23}^\circ + \varphi_{24}^\circ + \varphi_{25}^\circ + \\
& + \varphi_{26}^\circ + \varphi_{27}^\circ + \varphi_{28}^\circ + \varphi_{29}^\circ + \varphi_{30}^\circ + \varphi_{31}^\circ + \varphi_{40}^\circ + \varphi_{41}^\circ + \varphi_{42}^\circ + \varphi_{43}^\circ + \varphi_{44}^\circ + \varphi_{45}^\circ + \\
& + \varphi_{46}^\circ + \varphi_{47}^\circ + \varphi_{48}^\circ + \varphi_{49}^\circ + \varphi_{50}^\circ + \varphi_{51}^\circ + \varphi_{56}^\circ + \varphi_{57}^\circ + \varphi_{58}^\circ + \varphi_{59}^\circ + \varphi_{60}^\circ + \varphi_{61}^\circ) - \\
& - 3(\varphi_2^\circ + \varphi_3^\circ + \varphi_4^\circ + \varphi_5^\circ + \varphi_6^\circ + \varphi_7^\circ + \varphi_8^\circ + \varphi_9^\circ + \\
& + \varphi_{16}^\circ + \varphi_{17}^\circ + \varphi_{18}^\circ + \varphi_{19}^\circ + \varphi_{36}^\circ + \varphi_{37}^\circ + \varphi_{38}^\circ + \varphi_{39}^\circ + \\
& + \varphi_{32}^\circ + \varphi_{33}^\circ + \varphi_{34}^\circ + \varphi_{35}^\circ + \varphi_{52}^\circ + \varphi_{53}^\circ + \varphi_{54}^\circ + \varphi_{55}^\circ + \\
& + \varphi_{62}^\circ + \varphi_{63}^\circ + \varphi_{64}^\circ + \varphi_{65}^\circ + \varphi_{66}^\circ + \varphi_{67}^\circ + \varphi_{68}^\circ + \varphi_{69}^\circ)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_2} = \frac{\sqrt{3}}{36}\{ & 9(\varphi_2^\circ + \varphi_{69}^\circ) + \\
& + 2(\varphi_{13}^\circ + \varphi_{14}^\circ + \varphi_{15}^\circ + \varphi_{23}^\circ + \varphi_{24}^\circ + \varphi_{25}^\circ + \varphi_{26}^\circ + \varphi_{27}^\circ + \varphi_{28}^\circ + \varphi_{43}^\circ + \\
& + \varphi_{44}^\circ + \varphi_{45}^\circ + \varphi_{46}^\circ + \varphi_{47}^\circ + \varphi_{48}^\circ + \varphi_{56}^\circ + \varphi_{57}^\circ + \varphi_{58}^\circ) + \\
& + 1(\varphi_7^\circ + \varphi_8^\circ + \varphi_9^\circ + \varphi_{17}^\circ + \varphi_{18}^\circ + \varphi_{19}^\circ + \varphi_{32}^\circ + \varphi_{33}^\circ + \varphi_{34}^\circ + \varphi_{37}^\circ + \\
& + \varphi_{38}^\circ + \varphi_{39}^\circ + \varphi_{52}^\circ + \varphi_{53}^\circ + \varphi_{54}^\circ + \varphi_{62}^\circ + \varphi_{63}^\circ + \varphi_{64}^\circ) - \\
& - 3(\varphi_3^\circ + \varphi_4^\circ + \varphi_5^\circ + \varphi_6^\circ + \varphi_{16}^\circ + \varphi_{35}^\circ + \varphi_{36}^\circ + \varphi_{55}^\circ + \varphi_{65}^\circ + \varphi_{66}^\circ + \varphi_{67}^\circ + \varphi_{68}^\circ) - \\
& - 2(\varphi_{10}^\circ + \varphi_{11}^\circ + \varphi_{12}^\circ + \varphi_{20}^\circ + \varphi_{21}^\circ + \varphi_{22}^\circ + \varphi_{29}^\circ + \varphi_{30}^\circ + \varphi_{31}^\circ + \varphi_{40}^\circ \\
& \varphi_{41}^\circ + \varphi_{42}^\circ + \varphi_{49}^\circ + \varphi_{50}^\circ + \varphi_{51}^\circ + \varphi_{59}^\circ + \varphi_{60}^\circ + \varphi_{61}^\circ)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_3} = \frac{\sqrt{6}}{36}\{ & 6(\varphi_3^\circ + \varphi_{68}^\circ) + \\
& + 2(\varphi_{15}^\circ + \varphi_{25}^\circ + \varphi_{26}^\circ + \varphi_{45}^\circ + \varphi_{46}^\circ + \varphi_{56}^\circ) + \\
& + 1(\varphi_8^\circ + \varphi_9^\circ + \varphi_{11}^\circ + \varphi_{12}^\circ + \varphi_{18}^\circ + \varphi_{19}^\circ + \varphi_{21}^\circ + \varphi_{22}^\circ + \varphi_{29}^\circ + \varphi_{30}^\circ + \varphi_{32}^\circ + \varphi_{33}^\circ + \\
& + \varphi_{38}^\circ + \varphi_{39}^\circ + \varphi_{41}^\circ + \varphi_{42}^\circ + \varphi_{49}^\circ + \varphi_{50}^\circ + \varphi_{52}^\circ + \varphi_{53}^\circ + \varphi_{59}^\circ + \varphi_{60}^\circ + \varphi_{62}^\circ + \varphi_{63}^\circ) - \\
& - 3(\varphi_4^\circ + \varphi_5^\circ + \varphi_{66}^\circ + \varphi_{67}^\circ) - \\
& - 2(\varphi_7^\circ + \varphi_{10}^\circ + \varphi_{17}^\circ + \varphi_{20}^\circ + \varphi_{31}^\circ + \varphi_{34}^\circ + \varphi_{37}^\circ + \varphi_{40}^\circ + \varphi_{51}^\circ + \varphi_{54}^\circ + \varphi_{61}^\circ + \varphi_{64}^\circ) - \\
& - 1(\varphi_{13}^\circ + \varphi_{14}^\circ + \varphi_{23}^\circ + \varphi_{24}^\circ + \varphi_{27}^\circ + \varphi_{28}^\circ + \varphi_{43}^\circ + \varphi_{44}^\circ + \varphi_{47}^\circ + \varphi_{48}^\circ + \varphi_{57}^\circ + \varphi_{58}^\circ)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_4} = \frac{\sqrt{2}}{12}\{ & 3(\varphi^\circ_4 + \varphi^\circ_{67}) + \\
& +1(\varphi^\circ_9 + \varphi^\circ_{12} + \varphi^\circ_{14} + \varphi^\circ_{27} + \varphi^\circ_{29} + \varphi^\circ_{32} + \varphi^\circ_{19} + \varphi^\circ_{22} + \varphi^\circ_{24} + \varphi^\circ_{39} + \\
& + \varphi^\circ_{42} + \varphi^\circ_{44} + \varphi^\circ_{47} + \varphi^\circ_{49} + \varphi^\circ_{52} + \varphi^\circ_{57} + \varphi^\circ_{59} + \varphi^\circ_{62}) - \\
& -3(\varphi^\circ_5 + \varphi^\circ_{66}) - \\
& -1(\varphi^\circ_8 + \varphi^\circ_{11} + \varphi^\circ_{13} + \varphi^\circ_{18} + \varphi^\circ_{21} + \varphi^\circ_{23} + \varphi^\circ_{28} + \varphi^\circ_{30} + \varphi^\circ_{33} + \varphi^\circ_{38} + \\
& + \varphi^\circ_{41} + \varphi^\circ_{43} + \varphi^\circ_{48} + \varphi^\circ_{50} + \varphi^\circ_{53} + \varphi^\circ_{58} + \varphi^\circ_{60} + \varphi^\circ_{63})\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_5} = \frac{\sqrt{6}}{36}\{ & 6(\varphi^\circ_6 + \varphi^\circ_{65}) + \\
& +2(\varphi^\circ_{13} + \varphi^\circ_{14} + \varphi^\circ_{15} + \varphi^\circ_{56} + \varphi^\circ_{57} + \varphi^\circ_{58}) + \\
& +1(\varphi^\circ_{16} + \varphi^\circ_{17} + \varphi^\circ_{18} + \varphi^\circ_{20} + \varphi^\circ_{21} + \varphi^\circ_{22} + \varphi^\circ_{29} + \varphi^\circ_{30} + \varphi^\circ_{31} + \varphi^\circ_{32} + \varphi^\circ_{33} + \varphi^\circ_{34} + \\
& + \varphi^\circ_{37} + \varphi^\circ_{38} + \varphi^\circ_{39} + \varphi^\circ_{40} + \varphi^\circ_{41} + \varphi^\circ_{42} + \varphi^\circ_{49} + \varphi^\circ_{50} + \varphi^\circ_{51} + \varphi^\circ_{52} + \varphi^\circ_{53} + \varphi^\circ_{54}) - \\
& -3(\varphi^\circ_{16} + \varphi^\circ_{35} + \varphi^\circ_{55} + \varphi^\circ_{36}) - \\
& -2(\varphi^\circ_{10} + \varphi^\circ_{11} + \varphi^\circ_{12} + \varphi^\circ_7 + \varphi^\circ_8 + \varphi^\circ_9 + \varphi^\circ_{59} + \varphi^\circ_{60} + \varphi^\circ_{61} + \varphi^\circ_{62} + \varphi^\circ_{63} + \varphi^\circ_{64}) - \\
& -1(\varphi^\circ_{23} + \varphi^\circ_{24} + \varphi^\circ_{25} + \varphi^\circ_{26} + \varphi^\circ_{27} + \varphi^\circ_{28} + \varphi^\circ_{43} + \varphi^\circ_{44} + \varphi^\circ_{45} + \varphi^\circ_{46} + \varphi^\circ_{47} + \varphi^\circ_{48})\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_6} = \frac{\sqrt{3}}{36}\{ & 8(\varphi^\circ_7 + \varphi^\circ_{64}) + \\
& +4(\varphi^\circ_{15} + \varphi^\circ_{56}) \\
& +2(\varphi^\circ_{11} + \varphi^\circ_{12} + \varphi^\circ_{18} + \varphi^\circ_{19} + \varphi^\circ_{25} + \varphi^\circ_{31} + \varphi^\circ_{32} + \varphi^\circ_{33} + \\
& + \varphi^\circ_{38} + \varphi^\circ_{39} + \varphi^\circ_{45} + \varphi^\circ_{51} + \varphi^\circ_{59} + \varphi^\circ_{60}) + \\
& +1(\varphi^\circ_{23} + \varphi^\circ_{24} + \varphi^\circ_{27} + \varphi^\circ_{28} + \varphi^\circ_{43} + \varphi^\circ_{44} + \varphi^\circ_{47} + \varphi^\circ_{48}) - \\
& -4(\varphi^\circ_8 + \varphi^\circ_9 + \varphi^\circ_{10} + \varphi^\circ_{17} + \varphi^\circ_{34} + \varphi^\circ_{37} + \varphi^\circ_{54} + \varphi^\circ_{61}) - \\
& -2(\varphi^\circ_{13} + \varphi^\circ_{14} + \varphi^\circ_{25} + \varphi^\circ_{26} + \varphi^\circ_{45} + \varphi^\circ_{46} + \varphi^\circ_{52} + \varphi^\circ_{53} + \varphi^\circ_{57} + \varphi^\circ_{58}) - \\
& -1(\varphi^\circ_{21} + \varphi^\circ_{22} + \varphi^\circ_{29} + \varphi^\circ_{30} + \varphi^\circ_{41} + \varphi^\circ_{42} + \varphi^\circ_{49} + \varphi^\circ_{50})\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{S_7} = \frac{1}{12}\{ & 4(\varphi^\circ_8 + \varphi^\circ_{63}) + \\
& +2(\varphi^\circ_{12} + \varphi^\circ_{14} + \varphi^\circ_{19} + \varphi^\circ_{32} + \varphi^\circ_{39} + \varphi^\circ_{52} + \varphi^\circ_{57} + \varphi^\circ_{59}) +
\end{aligned}
$$

$$+1(\varphi_{21}^{\circ}+\varphi_{23}^{\circ}+\varphi_{28}^{\circ}+\varphi_{30}^{\circ}+\varphi_{41}^{\circ}+\varphi_{43}^{\circ}+\varphi_{48}^{\circ}+\varphi_{50}^{\circ})-$$
$$-4(\varphi_{9}^{\circ}+\varphi_{62}^{\circ})-$$
$$-2(\varphi_{11}^{\circ}+\varphi_{13}^{\circ}+\varphi_{18}^{\circ}+\varphi_{33}^{\circ}+\varphi_{38}^{\circ}+\varphi_{53}^{\circ}+\varphi_{58}^{\circ}+\varphi_{60}^{\circ})-$$
$$-1(\varphi_{22}^{\circ}+\varphi_{24}^{\circ}+\varphi_{27}^{\circ}+\varphi_{29}^{\circ}+\varphi_{42}^{\circ}+\varphi_{44}^{\circ}+\varphi_{47}^{\circ}+\varphi_{49}^{\circ})\}$$

$$\varphi_{S_8}=\frac{1}{12}\{4(\varphi_{10}^{\circ}+\varphi_{15}^{\circ}+\varphi_{56}^{\circ}+\varphi_{61}^{\circ})$$
$$+1(\varphi_{21}^{\circ}+\varphi_{22}^{\circ}+\varphi_{23}^{\circ}+\varphi_{24}^{\circ}+\varphi_{27}^{\circ}+\varphi_{28}^{\circ}+\varphi_{29}^{\circ}+\varphi_{30}^{\circ}+$$
$$+\varphi_{41}^{\circ}+\varphi_{42}^{\circ}+\varphi_{43}^{\circ}+\varphi_{44}^{\circ}+\varphi_{47}^{\circ}+\varphi_{48}^{\circ}+\varphi_{49}^{\circ}+\varphi_{50}^{\circ})-$$
$$-2(\varphi_{11}^{\circ}+\varphi_{12}^{\circ}+\varphi_{13}^{\circ}+\varphi_{14}^{\circ}+\varphi_{20}^{\circ}+\varphi_{25}^{\circ}+\varphi_{26}^{\circ}+\varphi_{31}^{\circ}+$$
$$+\varphi_{40}^{\circ}+\varphi_{45}^{\circ}+\varphi_{46}^{\circ}+\varphi_{51}^{\circ}+\varphi_{57}^{\circ}+\varphi_{58}^{\circ}+\varphi_{59}^{\circ}+\varphi_{60}^{\circ})\}$$

$$\varphi_{S_9}=\frac{\sqrt{3}}{12}\{2(\varphi_{11}^{\circ}+\varphi_{14}^{\circ}+\varphi_{57}^{\circ}+\varphi_{60}^{\circ})+$$
$$+1(\varphi_{22}^{\circ}+\varphi_{23}^{\circ}+\varphi_{28}^{\circ}+\varphi_{29}^{\circ}+\varphi_{42}^{\circ}+\varphi_{43}^{\circ}+\varphi_{48}^{\circ}+\varphi_{49}^{\circ})-$$
$$-2(\varphi_{12}^{\circ}+\varphi_{13}^{\circ}+\varphi_{58}^{\circ}+\varphi_{59}^{\circ})-$$
$$-1(\varphi_{21}^{\circ}+\varphi_{24}^{\circ}+\varphi_{27}^{\circ}+\varphi_{30}^{\circ}+\varphi_{41}^{\circ}+\varphi_{44}^{\circ}+\varphi_{47}^{\circ}+\varphi_{50}^{\circ})\}$$

$$\varphi_{S_{10}}=\frac{\sqrt{2}}{12}\{3(\varphi_{16}^{\circ}+\varphi_{55}^{\circ})+$$
$$+1(\varphi_{23}^{\circ}+\varphi_{24}^{\circ}+\varphi_{25}^{\circ}+\varphi_{29}^{\circ}+\varphi_{30}^{\circ}+\varphi_{31}^{\circ}+\varphi_{32}^{\circ}+\varphi_{33}^{\circ}+\varphi_{34}^{\circ}+\varphi_{37}^{\circ}+$$
$$+\varphi_{38}^{\circ}+\varphi_{39}^{\circ}+\varphi_{40}^{\circ}+\varphi_{41}^{\circ}+\varphi_{42}^{\circ}+\varphi_{46}^{\circ}+\varphi_{47}^{\circ}+\varphi_{48}^{\circ})-$$
$$-3(\varphi_{35}^{\circ}+\varphi_{36}^{\circ})$$
$$-1(\varphi_{17}^{\circ}+\varphi_{18}^{\circ}+\varphi_{19}^{\circ}+\varphi_{20}^{\circ}+\varphi_{21}^{\circ}+\varphi_{22}^{\circ}+\varphi_{26}^{\circ}+\varphi_{27}^{\circ}+\varphi_{28}^{\circ}+\varphi_{43}^{\circ}+$$
$$+\varphi_{44}^{\circ}+\varphi_{45}^{\circ}+\varphi_{49}^{\circ}+\varphi_{50}^{\circ}+\varphi_{51}^{\circ}+\varphi_{52}^{\circ}+\varphi_{53}^{\circ}+\varphi_{54}^{\circ})\}$$

$$\varphi_{S_{11}}=\frac{1}{12}\{4(\varphi_{17}^{\circ}+\varphi_{54}^{\circ}+\varphi_{55}^{\circ})+$$
$$+2(\varphi_{32}^{\circ}+\varphi_{33}^{\circ}+\varphi_{40}^{\circ}+\varphi_{45}^{\circ}+\varphi_{46}^{\circ}+\varphi_{51}^{\circ})+$$
$$+1(\varphi_{21}^{\circ}+\varphi_{22}^{\circ}+\varphi_{23}^{\circ}+\varphi_{24}^{\circ}+\varphi_{27}^{\circ}+\varphi_{28}^{\circ}+\varphi_{29}^{\circ}+\varphi_{30}^{\circ})-$$

$$-4\left(\varphi^{\circ}_{34}+\varphi^{\circ}_{35}+\varphi^{\circ}_{37}\right)-$$
$$-2\left(\varphi^{\circ}_{20}+\varphi^{\circ}_{25}+\varphi^{\circ}_{26}+\varphi^{\circ}_{31}+\varphi^{\circ}_{52}+\varphi^{\circ}_{53}\right)-$$
$$-1\left(\varphi^{\circ}_{41}+\varphi^{\circ}_{42}+\varphi^{\circ}_{43}+\varphi^{\circ}_{44}+\varphi^{\circ}_{47}+\varphi^{\circ}_{48}+\varphi^{\circ}_{49}+\varphi^{\circ}_{50}\right)\Big\}$$

$$\varphi_{S_{12}}=\frac{\sqrt{3}}{6}\Big\{2\left(\varphi^{\circ}_{18}+\varphi^{\circ}_{32}+\varphi^{\circ}_{39}+\varphi^{\circ}_{53}\right)+$$
$$+1\left(\varphi^{\circ}_{22}+\varphi^{\circ}_{24}+\varphi^{\circ}_{28}+\varphi^{\circ}_{30}+\varphi^{\circ}_{41}+\varphi^{\circ}_{43}+\varphi^{\circ}_{47}+\varphi^{\circ}_{49}\right)-$$
$$-2\left(\varphi^{\circ}_{19}+\varphi^{\circ}_{33}+\varphi^{\circ}_{38}+\varphi^{\circ}_{52}\right)-$$
$$-1\left(\varphi^{\circ}_{21}+\varphi^{\circ}_{23}+\varphi^{\circ}_{27}+\varphi^{\circ}_{29}+\varphi^{\circ}_{42}+\varphi^{\circ}_{44}+\varphi^{\circ}_{48}+\varphi^{\circ}_{50}\right)\Big\}$$

$$\varphi_{S_{13}}=\frac{\sqrt{3}}{24}\Big\{4\left(\varphi^{\circ}_{20}+\varphi^{\circ}_{25}+\varphi^{\circ}_{46}\right)+$$
$$+2\left(\varphi^{\circ}_{27}+\varphi^{\circ}_{28}+\varphi^{\circ}_{29}+\varphi^{\circ}_{30}+\varphi^{\circ}_{41}+\varphi^{\circ}_{42}+\varphi^{\circ}_{43}+\varphi^{\circ}_{44}\right)+$$
$$+1\left(\varphi^{\circ}_{51}\right)-$$
$$-4\left(\varphi^{\circ}_{26}+\varphi^{\circ}_{40}+\varphi^{\circ}_{45}\right)-$$
$$-2\left(\varphi^{\circ}_{21}+\varphi^{\circ}_{22}+\varphi^{\circ}_{23}+\varphi^{\circ}_{24}+\varphi^{\circ}_{47}+\varphi^{\circ}_{48}+\varphi^{\circ}_{49}+\varphi^{\circ}_{50}\right)-$$
$$-1\left(\varphi^{\circ}_{31}\right)\Big\}$$

$$\varphi_{S_{14}}=\frac{1}{4}\Big\{+1\left(\varphi^{\circ}_{21}+\varphi^{\circ}_{24}+\varphi^{\circ}_{28}+\varphi^{\circ}_{29}+\varphi^{\circ}_{42}+\varphi^{\circ}_{43}+\varphi^{\circ}_{47}+\varphi^{\circ}_{50}\right)-$$
$$-1\left(\varphi^{\circ}_{22}+\varphi^{\circ}_{23}+\varphi^{\circ}_{27}+\varphi^{\circ}_{30}+\varphi^{\circ}_{41}+\varphi^{\circ}_{44}+\varphi^{\circ}_{48}+\varphi^{\circ}_{49}\right)\Big\}$$

B./ Triplettek

Az 1 eredő spinhez tartozó SLATER- determinánsokat a következőképpen jelöljük :

$\varphi_{1}^{1} = |\alpha\alpha\alpha\alpha\alpha\beta\beta\beta|$

$\varphi_{2}^{1} = |\alpha\alpha\alpha\alpha\beta\alpha\beta\beta|$

$\varphi_{3}^{1} = |\alpha\alpha\alpha\alpha\beta\beta\alpha\beta|$

$\varphi_{4}^{1} = |\alpha\alpha\alpha\alpha\beta\beta\beta\alpha|$

$\varphi_{5}^{1} = |\alpha\alpha\alpha\beta\alpha\alpha\beta\beta|$

$\varphi_{6}^{1} = |\alpha\alpha\alpha\beta\alpha\beta\alpha\beta|$

$\varphi_{7}^{1} = |\alpha\alpha\alpha\beta\alpha\beta\beta\alpha|$

$\varphi_{8}^{1} = |\alpha\alpha\alpha\beta\beta\alpha\alpha\beta|$

$\varphi_{9}^{1} = |\alpha\alpha\alpha\beta\beta\alpha\beta\alpha|$

$\varphi_{10}^{1} = |\alpha\alpha\alpha\beta\beta\beta\alpha\alpha|$

$\varphi_{11}^{1} = |\alpha\alpha\beta\alpha\alpha\alpha\beta\beta|$

$\varphi_{12}^{1} = |\alpha\alpha\beta\alpha\alpha\beta\alpha\beta|$

$\varphi_{13}^{1} = |\alpha\alpha\beta\alpha\alpha\beta\beta\alpha|$

$\varphi_{14}^{1} = |\alpha\alpha\beta\alpha\beta\alpha\alpha\beta|$

$\varphi_{15}^{1} = |\alpha\alpha\beta\alpha\beta\alpha\beta\alpha|$

$\varphi_{16}^{1} = |\alpha\alpha\beta\alpha\beta\beta\alpha\alpha|$

$\varphi_{17}^{1} = |\alpha\alpha\beta\beta\alpha\alpha\alpha\beta|$

$\varphi_{18}^{1} = |\alpha\alpha\beta\beta\alpha\alpha\beta\alpha|$

$\varphi_{19}^{1} = |\alpha\alpha\beta\beta\alpha\beta\alpha\alpha|$

$\varphi_{20}^{1} = |\alpha\alpha\beta\beta\beta\alpha\alpha\alpha|$

$\varphi_{21}^{1} = |\alpha\beta\alpha\alpha\alpha\alpha\beta\beta|$

$\varphi_{22}^{1} = |\alpha\beta\alpha\alpha\alpha\beta\alpha\beta|$

$\varphi_{23}^{1} = |\alpha\beta\alpha\alpha\alpha\beta\beta\alpha|$

$\varphi_{24}^{1} = |\alpha\beta\alpha\alpha\beta\alpha\alpha\beta|$

$\varphi_{25}^{1} = |\alpha\beta\alpha\alpha\beta\alpha\beta\alpha|$

$\varphi_{26}^{1} = |\alpha\beta\alpha\alpha\beta\beta\alpha\alpha|$

$\varphi_{27}^{1} = |\alpha\beta\alpha\beta\alpha\alpha\alpha\beta|$

$\varphi_{28}^{1} = |\alpha\beta\alpha\beta\alpha\alpha\beta\alpha|$

$\varphi_{29}^{1} = |\alpha\beta\alpha\beta\alpha\beta\alpha\alpha|$

$\varphi_{30}^{1} = |\alpha\beta\alpha\beta\beta\alpha\alpha\alpha|$

$\varphi_{31}^{1} = |\alpha\beta\beta\alpha\alpha\alpha\alpha\beta|$

$\varphi_{32}^{1} = |\alpha\beta\beta\alpha\alpha\alpha\beta\alpha|$

$\varphi_{33}^{1} = |\alpha\beta\beta\alpha\alpha\beta\alpha\alpha|$

$\varphi_{34}^{1} = |\alpha\beta\beta\alpha\beta\alpha\alpha\alpha|$

$\varphi_{35}^{1} = |\alpha\beta\beta\beta\alpha\alpha\alpha\alpha|$

$\varphi_{36}^{1} = |\beta\alpha\alpha\alpha\alpha\alpha\beta\beta|$

$\varphi_{37}^{1} = |\beta\alpha\alpha\alpha\alpha\beta\alpha\beta|$

$\varphi_{38}^{1} = |\beta\alpha\alpha\alpha\alpha\beta\beta\alpha|$

$\varphi_{39}^{1} = |\beta\alpha\alpha\alpha\beta\alpha\alpha\beta|$

$\varphi_{40}^{1} = |\beta\alpha\alpha\alpha\beta\alpha\beta\alpha|$

$\varphi_{41}^{1} = |\beta\alpha\alpha\alpha\beta\beta\alpha\alpha|$

$\varphi_{42}^{1} = |\beta\alpha\alpha\beta\alpha\alpha\alpha\beta|$

$\varphi_{43}^{1} = |\beta\alpha\alpha\beta\alpha\alpha\beta\alpha|$

$\varphi_{44}^{1} = |\beta\alpha\alpha\beta\alpha\beta\alpha\alpha|$

$\varphi_{45}^{1} = |\beta\alpha\alpha\beta\beta\alpha\alpha\alpha|$

$\varphi_{46}^{1} = |\beta\alpha\beta\alpha\alpha\alpha\alpha\beta|$

$\varphi_{47}^{1} = |\beta\alpha\beta\alpha\alpha\alpha\beta\alpha|$

$\varphi_{48}^{1} = |\beta\alpha\beta\alpha\alpha\beta\alpha\alpha|$

$\varphi_{49}^{1} = |\beta\alpha\beta\alpha\beta\alpha\alpha\alpha|$

$\varphi_{50}^{1} = |\beta\alpha\beta\beta\alpha\alpha\alpha\alpha|$

$\varphi_{51}^{1} = |\beta\beta\alpha\alpha\alpha\alpha\alpha\beta|$

$\varphi_{52}^{1} = |\beta\beta\alpha\alpha\alpha\alpha\beta\alpha|$

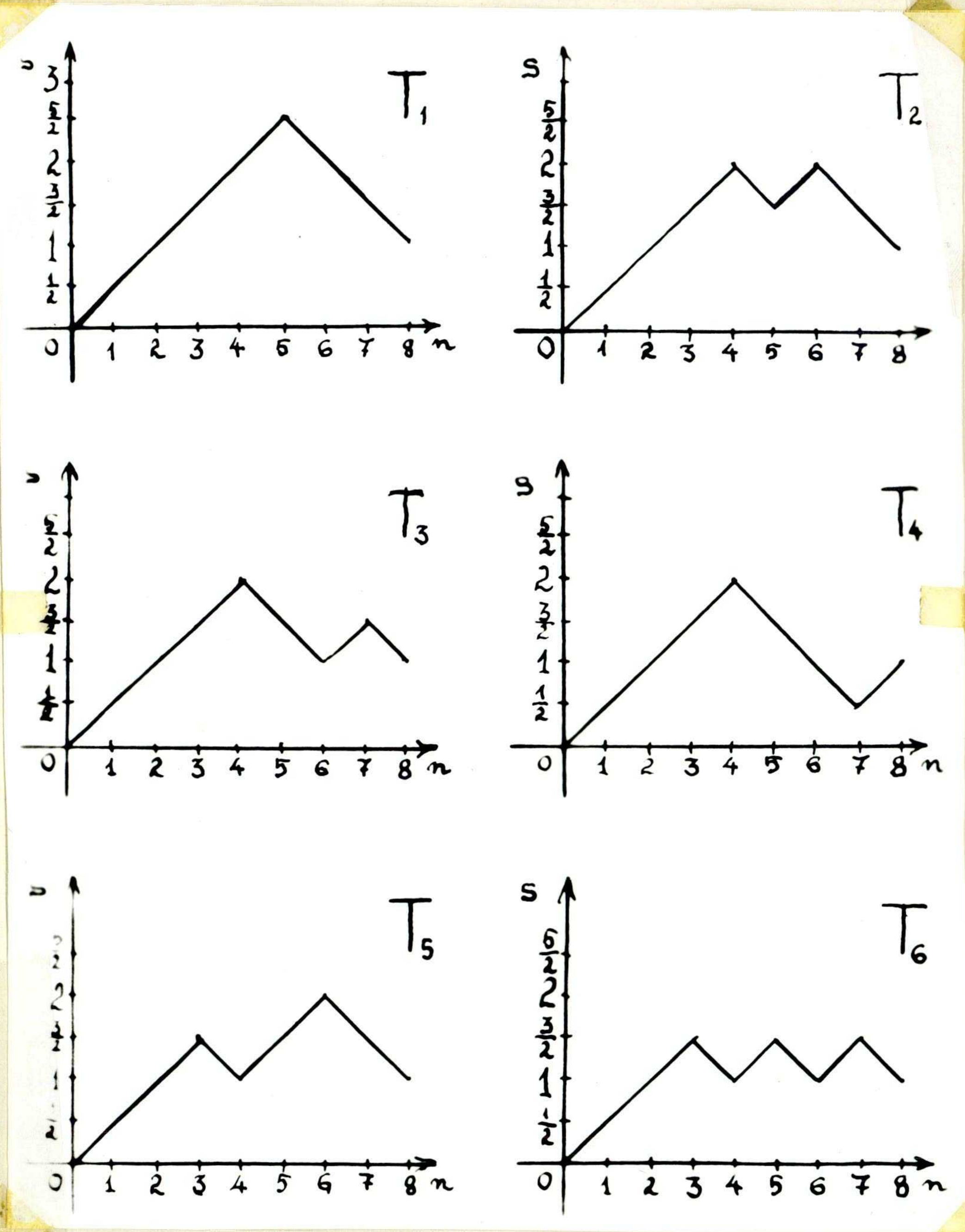
$\varphi_{53}^{1} = |\beta\beta\alpha\alpha\alpha\beta\alpha\alpha|$

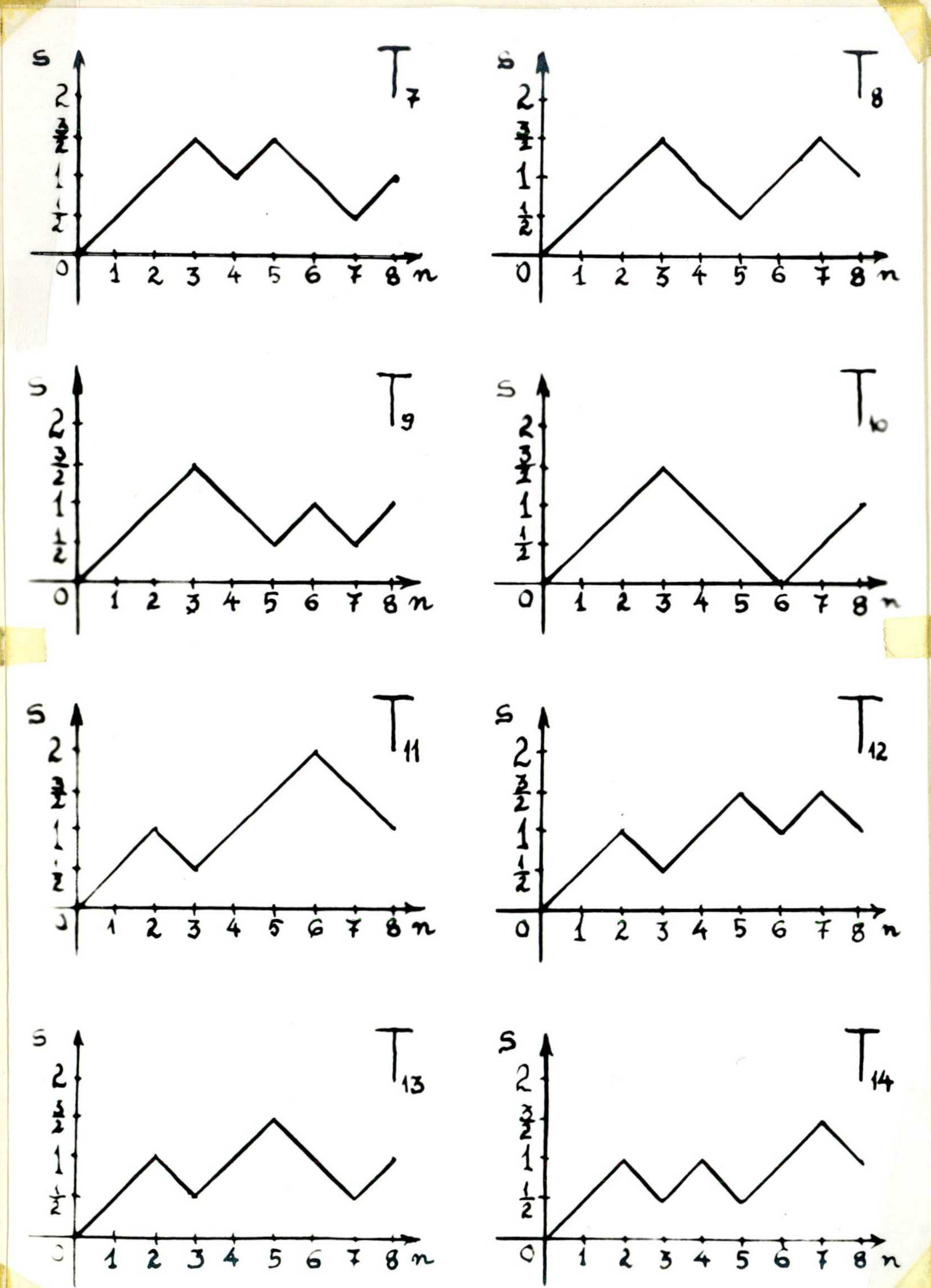
$\varphi_{54}^{1} = |\beta\beta\alpha\alpha\beta\alpha\alpha\alpha|$

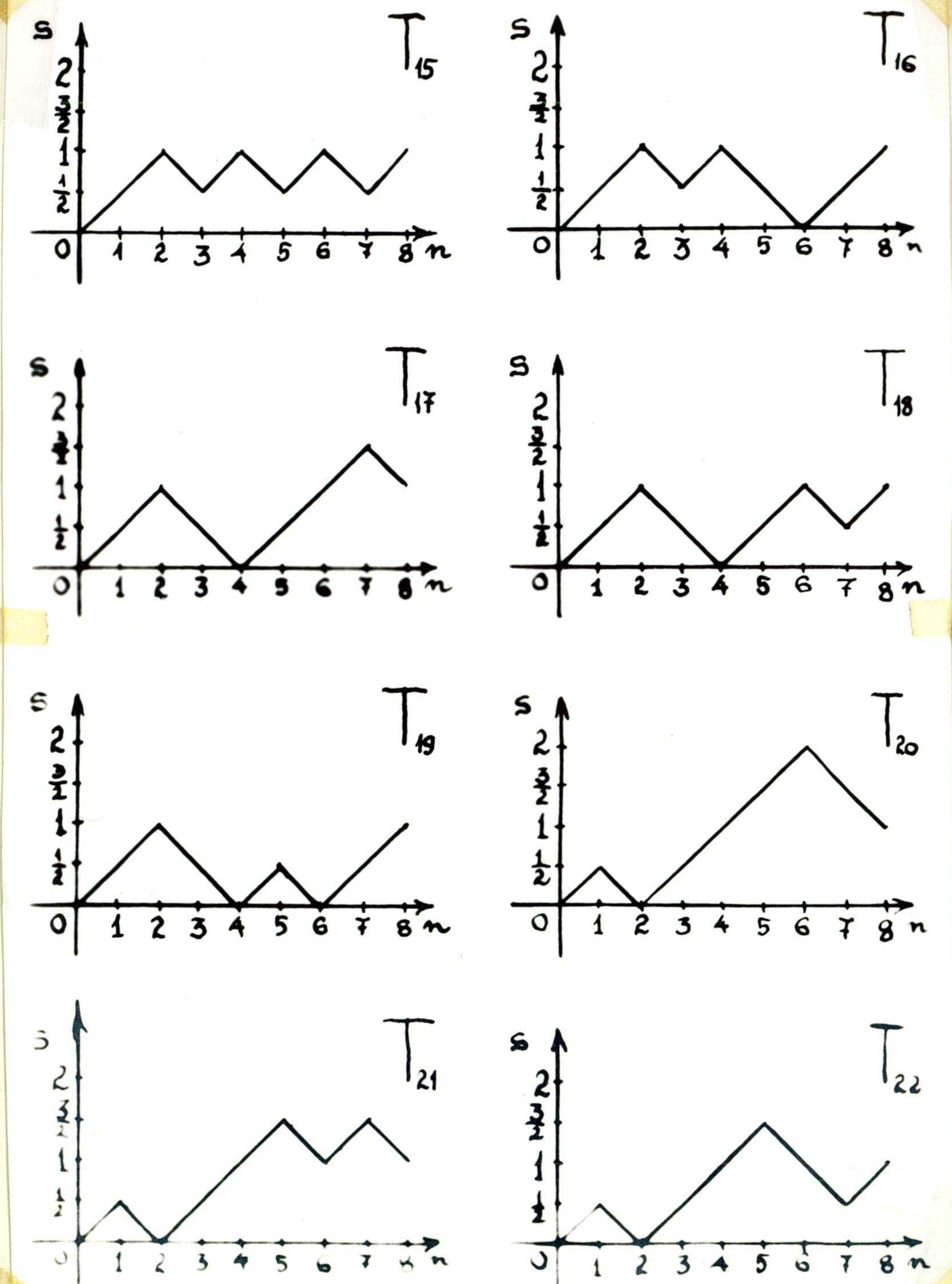
$\varphi_{55}^{1} = |\beta\beta\alpha\beta\alpha\alpha\alpha\alpha|$

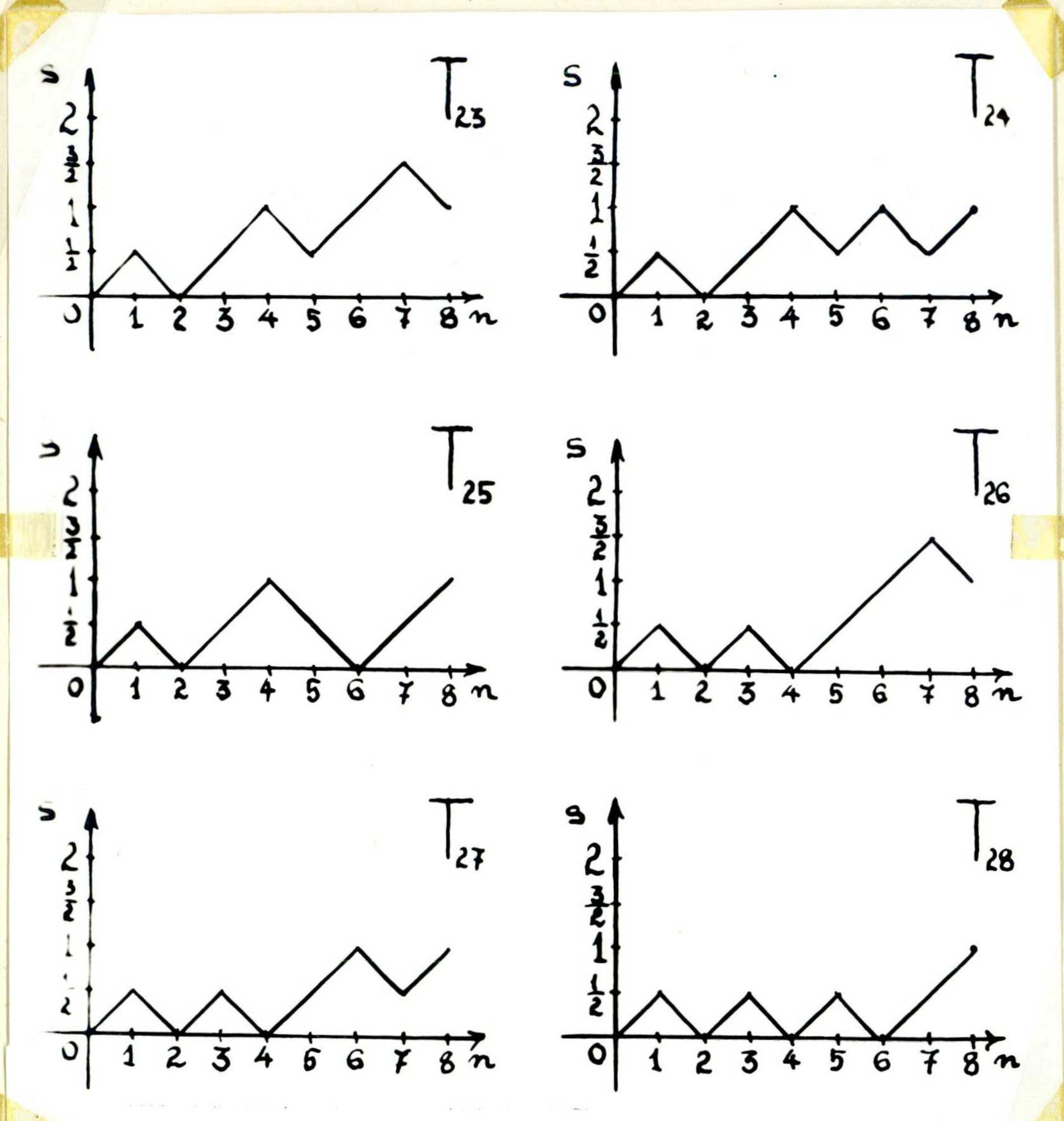
$\varphi_{56}^{1} = |\beta\beta\beta\alpha\alpha\alpha\alpha\alpha|$

Tripletteket az elágazási diagram szerint 28 féleképpen szerkeszthetünk :




T7
T8
T9
T10
T11
T12
T13
T14
s
n


T15
T16
T17
T18
T19
T20
T21
T22



A megfelelő sajátfüggvények a következők :

$$\varphi_{T_1} = \frac{\sqrt{2}}{20}\{10\,(\varphi_1^1) +$$
$$+1\,(\varphi_8^1 + \varphi_9^1 + \varphi_{10}^1 + \varphi_{14}^1 + \varphi_{15}^1 + \varphi_{16}^1 + \varphi_{17}^1 + \varphi_{18}^1 + \varphi_{19}^1 + \varphi_{24}^1 +$$

$$+\varphi^1_{25}+\varphi^1_{26}+\varphi^1_{27}+\varphi^1_{28}+\varphi^1_{29}+\varphi^1_{31}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{39}+\varphi^1_{40}+$$
$$+\varphi^1_{41}+\varphi^1_{42}+\varphi^1_{43}+\varphi^1_{44}+\varphi^1_{46}+\varphi^1_{47}+\varphi^1_{48}+\varphi^1_{51}+\varphi^1_{52}+\varphi^1_{53})-$$
$$-2(\varphi^1_{2}+\varphi^1_{3}+\varphi^1_{4}+\varphi^1_{5}+\varphi^1_{6}+\varphi^1_{7}+\varphi^1_{11}+\varphi^1_{12}+$$
$$+\varphi^1_{13}+\varphi^1_{21}+\varphi^1_{22}+\varphi^1_{23}+\varphi^1_{36}+\varphi^1_{37}+\varphi^1_{38})-$$
$$-1(\varphi^1_{20}+\varphi^1_{30}+\varphi^1_{34}+\varphi^1_{35}+\varphi^1_{45}+\varphi^1_{49}+\varphi^1_{50}+\varphi^1_{54}+\varphi^1_{55}+\varphi^1_{56})\}$$

$$\varphi_{T_2}=\frac{\sqrt{3}}{120}\{48(\varphi^1_{2})+$$
$$+6(\varphi^1_{17}+\varphi^1_{18}+\varphi^1_{27}+\varphi^1_{28}+\varphi^1_{31}+\varphi^1_{32}+\varphi^1_{42}+\varphi^1_{43}+$$
$$+\varphi^1_{46}+\varphi^1_{47}+\varphi^1_{51}+\varphi^1_{52}+\varphi^1_{10}+\varphi^1_{16}+\varphi^1_{26}+\varphi^1_{41})+$$
$$+4(\varphi^1_{20}+\varphi^1_{30}+\varphi^1_{34}+\varphi^1_{45}+\varphi^1_{49}+\varphi^1_{54})+$$
$$+3(\varphi^1_{6}+\varphi^1_{7}+\varphi^1_{12}+\varphi^1_{13}+\varphi^1_{22}+\varphi^1_{23}+\varphi^1_{37}+\varphi^1_{38})-$$
$$-12(\varphi^1_{3}+\varphi^1_{4}+\varphi^1_{5}+\varphi^1_{11}+\varphi^1_{21}+\varphi^1_{36})-$$
$$-9(\varphi^1_{8}+\varphi^1_{9}+\varphi^1_{14}+\varphi^1_{15}+\varphi^1_{24}+\varphi^1_{25}+\varphi^1_{39}+\varphi^1_{40})-$$
$$-6(\varphi^1_{35}+\varphi^1_{50}+\varphi^1_{55}+\varphi^1_{56})-$$
$$-4(\varphi^1_{19}+\varphi^1_{29}+\varphi^1_{33}+\varphi^1_{44}+\varphi^1_{48}+\varphi^1_{53})\}$$

$$\varphi_{T_3}=\frac{\sqrt{5}}{120}\{36(\varphi^1_{3})+$$
$$+6(\varphi^1_{17}+\varphi^1_{27}+\varphi^1_{31}+\varphi^1_{42}+\varphi^1_{46}+\varphi^1_{51})+$$
$$+4(\varphi^1_{19}+\varphi^1_{20}+\varphi^1_{29}+\varphi^1_{30}+\varphi^1_{33}+\varphi^1_{34}+\varphi^1_{44}+\varphi^1_{45}+\varphi^1_{48}+\varphi^1_{49}+\varphi^1_{53}+\varphi^1_{54})+$$
$$+3(\varphi^1_{7}+\varphi^1_{9}+\varphi^1_{13}+\varphi^1_{15}+\varphi^1_{23}+\varphi^1_{25}+\varphi^1_{38}+\varphi^1_{40})-$$
$$-12(\varphi^1_{4})-$$
$$-9(\varphi^1_{6}+\varphi^1_{8}+\varphi^1_{12}+\varphi^1_{14}+\varphi^1_{22}+\varphi^1_{24}+\varphi^1_{37}+\varphi^1_{39})-$$
$$-6(\varphi^1_{10}+\varphi^1_{16}+\varphi^1_{26}+\varphi^1_{35}+\varphi^1_{41}+\varphi^1_{50}+\varphi^1_{55}+\varphi^1_{56})-$$
$$-2(\varphi^1_{18}+\varphi^1_{28}+\varphi^1_{32}+\varphi^1_{43}+\varphi^1_{47}+\varphi^1_{52})\}$$

$$\varphi_{T_4}=\frac{\sqrt{10}}{60}\{12(\varphi^1_{4})+$$
$$2(\varphi^1_{18}+\varphi^1_{19}+\varphi^1_{20}+\varphi^1_{28}+\varphi^1_{29}+\varphi^1_{30}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{34}+\varphi^1_{43}+$$

$$+\varphi^1_{44}+\varphi^1_{45}+\varphi^1_{47}+\varphi^1_{48}+\varphi^1_{49}+\varphi^1_{52}+\varphi^1_{53}+\varphi^1_{54})-$$
$$-3(\varphi^1_{7}+\varphi^1_{9}+\varphi^1_{10}+\varphi^1_{13}+\varphi^1_{15}+\varphi^1_{16}+\varphi^1_{23}+\varphi^1_{25}+$$
$$+\varphi^1_{26}+\varphi^1_{35}+\varphi^1_{38}+\varphi^1_{40}+\varphi^1_{41}+\varphi^1_{50}+\varphi^1_{55}+\varphi^1_{56})\}$$

$$\varphi_{T_5}=\frac{\sqrt{5}}{120}\{36(\varphi^1_5)+$$
$$+6(\varphi^1_{10}+\varphi^1_{31}+\varphi^1_{32}+\varphi^1_{46}+\varphi^1_{47}+\varphi^1_{51}+\varphi^1_{52})+$$
$$+4(\varphi^1_{19}+\varphi^1_{20}+\varphi^1_{29}+\varphi^1_{30}+\varphi^1_{44}+\varphi^1_{45})+$$
$$+3(\varphi^1_{12}+\varphi^1_{13}+\varphi^1_{14}+\varphi^1_{15}+\varphi^1_{22}+\varphi^1_{23}+\varphi^1_{24}+\varphi^1_{25}+\varphi^1_{37}+\varphi^1_{38}+\varphi^1_{39}+\varphi^1_{40})+$$
$$+2(\varphi^1_{35}+\varphi^1_{50}+\varphi^1_{55})-$$
$$-12(\varphi^1_{11}+\varphi^1_{21}+\varphi^1_{36})-$$
$$-9(\varphi^1_{6}+\varphi^1_{7}+\varphi^1_{8}+\varphi^1_{9})-$$
$$-6(\varphi^1_{17}+\varphi^1_{18}+\varphi^1_{27}+\varphi^1_{28}+\varphi^1_{42}+\varphi^1_{43}+\varphi^1_{56})-$$
$$-4(\varphi^1_{33}+\varphi^1_{34}+\varphi^1_{48}+\varphi^1_{49}+\varphi^1_{53}+\varphi^1_{54})-$$
$$-2(\varphi^1_{16}+\varphi^1_{26}+\varphi^1_{41})\}$$

$$\varphi_{T_6}=\frac{\sqrt{3}}{72}\{27(\varphi^1_6)+$$
$$+6(\varphi^1_{31}+\varphi^1_{46}+\varphi^1_{51})+$$
$$+4(\varphi^1_{20}+\varphi^1_{30}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{48}+\varphi^1_{53})+$$
$$+3(\varphi^1_{9}+\varphi^1_{13}+\varphi^1_{14}+\varphi^1_{23}+\varphi^1_{24}+\varphi^1_{38}+\varphi^1_{39})+$$
$$+2(\varphi^1_{16}+\varphi^1_{18}+\varphi^1_{26}+\varphi^1_{28}+\varphi^1_{35}+\varphi^1_{41}+\varphi^1_{43}+\varphi^1_{50}+\varphi^1_{55})-$$
$$-9(\varphi^1_{7}+\varphi^1_{8}+\varphi^1_{12}+\varphi^1_{22}+\varphi^1_{37})-$$
$$-6(\varphi^1_{10}+\varphi^1_{17}+\varphi^1_{27}+\varphi^1_{42}+\varphi^1_{56})-$$
$$-4(\varphi^1_{19}+\varphi^1_{29}+\varphi^1_{34}+\varphi^1_{44}+\varphi^1_{49}+\varphi^1_{54})-$$
$$-2(\varphi^1_{32}+\varphi^1_{47}+\varphi^1_{52})-$$
$$-1(\varphi^1_{15}+\varphi^1_{25}+\varphi^1_{40})\}$$

$$\varphi_{T_7} = \frac{\sqrt{6}}{36}\{9(\varphi_7^1) +$$
$$+2(\varphi_{20}^1 + \varphi_{30}^1 + \varphi_{32}^1 + \varphi_{33}^1 + \varphi_{45}^1 + \varphi_{47}^1 + \varphi_{48}^1 + \varphi_{52}^1 + \varphi_{53}^1) +$$
$$+1(\varphi_{15}^1 + \varphi_{16}^1 + \varphi_{25}^1 + \varphi_{26}^1 + \varphi_{35}^1 + \varphi_{40}^1 + \varphi_{41}^1 + \varphi_{50}^1 + \varphi_{55}^1) -$$
$$-3(\varphi_9^1 + \varphi_{10}^1 + \varphi_{13}^1 + \varphi_{23}^1 + \varphi_{38}^1 + \varphi_{56}^1) -$$
$$-2(\varphi_{18}^1 + \varphi_{19}^1 + \varphi_{28}^1 + \varphi_{29}^1 + \varphi_{43}^1 + \varphi_{44}^1 + \varphi_{34}^1 + \varphi_{49}^1 + \varphi_{54}^1)\}$$

$$\varphi_{T_8} = \frac{\sqrt{6}}{36}\{9(\varphi_8^1) +$$
$$+2(\varphi_{20}^1 + \varphi_{30}^1 + \varphi_{45}^1) +$$
$$+1(\varphi_{15}^1 + \varphi_{16}^1 + \varphi_{18}^1 + \varphi_{19}^1 + \varphi_{25}^1 + \varphi_{26}^1 + \varphi_{28}^1 + \varphi_{29}^1 + \varphi_{34}^1 +$$
$$+ \varphi_{35}^1 + \varphi_{40}^1 + \varphi_{41}^1 + \varphi_{43}^1 + \varphi_{44}^1 + \varphi_{49}^1 + \varphi_{50}^1 + \varphi_{54}^1 + \varphi_{55}^1) -$$
$$-3(\varphi_9^1 + \varphi_{10}^1 + \varphi_{14}^1 + \varphi_{20}^1 + \varphi_{24}^1 + \varphi_{30}^1 + \varphi_{39}^1 + \varphi_{45}^1 + \varphi_{56}^1) -$$
$$-1(\varphi_{32}^1 + \varphi_{33}^1 + \varphi_{47}^1 + \varphi_{48}^1 + \varphi_{52}^1 + \varphi_{53}^1)\}$$

$$\varphi_{T_9} = \frac{\sqrt{3}}{18}\{6(\varphi_9^1) +$$
$$+2(\varphi_{32}^1 + \varphi_{47}^1 + \varphi_{52}^1) +$$
$$+1(\varphi_{16}^1 + \varphi_{19}^1 + \varphi_{26}^1 + \varphi_{29}^1 + \varphi_{34}^1 + \varphi_{35}^1 + \varphi_{41}^1 + \varphi_{44}^1 + \varphi_{49}^1 + \varphi_{50}^1 + \varphi_{54}^1 + \varphi_{55}^1) -$$
$$-3(\varphi_{10}^1 + \varphi_{56}^1) -$$
$$-2(\varphi_{15}^1 + \varphi_{18}^1 + \varphi_{25}^1 + \varphi_{28}^1 + \varphi_{40}^1 + \varphi_{43}^1) -$$
$$-1(\varphi_{20}^1 + \varphi_{30}^1 + \varphi_{33}^1 + \varphi_{45}^1 + \varphi_{48}^1 + \varphi_{53}^1)\}$$

$$\varphi_{T_{10}} = \frac{1}{6}\{3(\varphi_{10}^1) +$$
$$+1(\varphi_{33}^1 + \varphi_{34}^1 + \varphi_{35}^1 + \varphi_{18}^1 + \varphi_{49}^1 + \varphi_{50}^1 + \varphi_{55}^1 + \varphi_{53}^1 + \varphi_{54}^1) -$$
$$-3(\varphi_{56}^1) -$$
$$-1(\varphi_{16}^1 + \varphi_{19}^1 + \varphi_{20}^1 + \varphi_{29}^1 + \varphi_{30}^1 + \varphi_{26}^1 + \varphi_{41}^1 + \varphi_{44}^1 + \varphi_{45}^1)\}$$

$$\varphi_{T_{11}} = \frac{\sqrt{10}}{120}\{24(\varphi_{11}^1) +$$
$$+6(\varphi_{51}^1 + \varphi_{52}^1) +$$

$$+4(\varphi_{16}^{1}+\varphi_{19}^{1}+\varphi_{20}^{1})+$$
$$+3(\varphi_{22}^{1}+\varphi_{23}^{1}+\varphi_{24}^{1}+\varphi_{25}^{1}+\varphi_{27}^{1}+\varphi_{28}^{1}+\varphi_{37}^{1}+\varphi_{38}^{1}+\varphi_{39}^{1}+\varphi_{40}^{1}+\varphi_{42}^{1}+\varphi_{43}^{1})+$$
$$+2(\varphi_{33}^{1}+\varphi_{34}^{1}+\varphi_{35}^{1}+\varphi_{48}^{1}+\varphi_{49}^{1}+\varphi_{50}^{1})-$$
$$-12(\varphi_{21}^{1}+\varphi_{36}^{1})-$$
$$-6(\varphi_{12}^{1}+\varphi_{13}^{1}+\varphi_{14}^{1}+\varphi_{15}^{1}+\varphi_{17}^{1}+\varphi_{18}^{1})-$$
$$-4(\varphi_{53}^{1}+\varphi_{54}^{1}+\varphi_{55}^{1})-$$
$$-3(\varphi_{31}^{1}+\varphi_{32}^{1}+\varphi_{46}^{1}+\varphi_{47}^{1})-$$
$$-2(\varphi_{26}^{1}+\varphi_{29}^{1}+\varphi_{30}^{1}+\varphi_{41}^{1}+\varphi_{44}^{1}+\varphi_{45}^{1})\}$$

$$\varphi_{T_{12}}=\frac{\sqrt{6}}{72}\{18(\varphi_{12}^{1})+$$
$$+6(\varphi_{51}^{1})+$$
$$+4(\varphi_{20}^{1}+\varphi_{53}^{1})+$$
$$+3(\varphi_{23}^{1}+\varphi_{24}^{1}+\varphi_{27}^{1}+\varphi_{38}^{1}+\varphi_{39}^{1}+\varphi_{42}^{1})+$$
$$+2(\varphi_{15}^{1}+\varphi_{18}^{1}+\varphi_{26}^{1}+\varphi_{29}^{1}+\varphi_{34}^{1}+\varphi_{35}^{1}+\varphi_{41}^{1}+\varphi_{44}^{1}+\varphi_{49}^{1}+\varphi_{50}^{1})$$
$$+1(\varphi_{32}^{1}+\varphi_{47}^{1})-$$
$$-9(\varphi_{22}^{1}+\varphi_{37}^{1})-$$
$$-6(\varphi_{13}^{1}+\varphi_{14}^{1}+\varphi_{17}^{1})-$$
$$-4(\varphi_{16}^{1}+\varphi_{19}^{1}+\varphi_{54}^{1}+\varphi_{55}^{1})$$
$$-3(\varphi_{31}^{1}+\varphi_{46}^{1})-$$
$$-2(\varphi_{30}^{1}+\varphi_{33}^{1}+\varphi_{45}^{1}+\varphi_{48}^{1}+\varphi_{52}^{1})-$$
$$-1(\varphi_{25}^{1}+\varphi_{28}^{1}+\varphi_{40}^{1}+\varphi_{43}^{1})\}$$

$$\varphi_{T_{13}}=\frac{\sqrt{3}}{3}\{6(\varphi_{13}^{1})+$$
$$+2(\varphi_{20}^{1}+\varphi_{52}^{1}+\varphi_{53}^{1})+$$
$$+1(\varphi_{25}^{1}+\varphi_{26}^{1}+\varphi_{28}^{1}+\varphi_{29}^{1}+\varphi_{34}^{1}+\varphi_{35}^{1}+\varphi_{40}^{1}+\varphi_{41}^{1}+\varphi_{43}^{1}+\varphi_{44}^{1}+\varphi_{49}^{1}+\varphi_{50}^{1})-$$
$$-3(\varphi_{23}^{1}+\varphi_{38}^{1})-$$

$$-2(\varphi^1_{15}+\varphi^1_{16}+\varphi^1_{18}+\varphi^1_{19}+\varphi^1_{54}+\varphi^1_{55})-$$
$$-1(\varphi^1_{30}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{47}+\varphi^1_{48})\}$$

$$\varphi_{T_{14}}=\frac{\sqrt{3}}{36}\{12(\varphi^1_{14})+$$
$$+6(\varphi^1_{51})+$$
$$+3(\varphi^1_{27}+\varphi^1_{42})+$$
$$+2(\varphi^1_{18}+\varphi^1_{19}+\varphi^1_{25}+\varphi^1_{26}+\varphi^1_{35}+\varphi^1_{40}+\varphi^1_{41}+\varphi^1_{50}+\varphi^1_{54})+$$
$$+1(\varphi^1_{30}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{43}+\varphi^1_{47}+\varphi^1_{48})-$$
$$-6(\varphi^1_{17}+\varphi^1_{24}+\varphi^1_{39})-$$
$$-4(\varphi^1_{15}+\varphi^1_{16}+\varphi^1_{55})-$$
$$-3(\varphi^1_{31}+\varphi^1_{46})-$$
$$-2(\varphi^1_{20}+\varphi^1_{52}+\varphi^1_{53})-$$
$$-1(\varphi^1_{28}+\varphi^1_{29}+\varphi^1_{34}+\varphi^1_{43}+\varphi^1_{44}+\varphi^1_{49})\}$$

$$\varphi_{T_{15}}=\frac{\sqrt{6}}{36}\{8(\varphi^1_{15})+$$
$$+4(\varphi^1_{52})+$$
$$+2(\varphi^1_{19}+\varphi^1_{26}+\varphi^1_{28}+\varphi^1_{32}+\varphi^1_{35}+\varphi^1_{41}+\varphi^1_{48}+\varphi^1_{50}+\varphi^1_{54})+$$
$$+1(\varphi^1_{30}+\varphi^1_{33}+\varphi^1_{45})-$$
$$-4(\varphi^1_{16}+\varphi^1_{18}+\varphi^1_{25}+\varphi^1_{40}+\varphi^1_{55})-$$
$$-2(\varphi^1_{20}+\varphi^1_{43}+\varphi^1_{47}+\varphi^1_{53})-$$
$$-1(\varphi^1_{29}+\varphi^1_{34}+\varphi^1_{44}+\varphi^1_{48}+\varphi^1_{49})\}$$

$$\varphi_{T_{16}}=\frac{\sqrt{2}}{12}\{4(\varphi^1_{16})+$$
$$+2(\varphi^1_{35}+\varphi^1_{50}+\varphi^1_{53}+\varphi^1_{54})+$$
$$+1(\varphi^1_{29}+\varphi^1_{30}+\varphi^1_{44}+\varphi^1_{45})-$$
$$-4(\varphi^1_{55})-$$

$$-2(\varphi'_{19}+\varphi'_{20}+\varphi'_{26}+\varphi'_{41})$$
$$-1(\varphi'_{33}+\varphi'_{34}+\varphi'_{48}+\varphi'_{49})\}$$

$$\varphi_{T_{17}}=\frac{1}{12}\{6(\varphi'_{17}+\varphi'_{51})+$$
$$+1(\varphi'_{28}+\varphi'_{29}+\varphi'_{30}+\varphi'_{32}+\varphi'_{33}+\varphi'_{34}+\varphi'_{43}+\varphi'_{44}+\varphi'_{45}+\varphi'_{47}+\varphi'_{48}+\varphi'_{49})-$$
$$-2(\varphi'_{18}+\varphi'_{19}+\varphi'_{20}+\varphi'_{52}+\varphi'_{53}+\varphi'_{54})-$$
$$-3(\varphi'_{27}+\varphi'_{31}+\varphi'_{42}+\varphi'_{46})\}$$

$$\varphi_{T_{18}}=\frac{\sqrt{2}}{12}\{4(\varphi'_{18}+\varphi'_{52})+$$
$$+1(\varphi'_{29}+\varphi'_{30}+\varphi'_{33}+\varphi'_{34}+\varphi'_{44}+\varphi'_{45}+\varphi'_{48}+\varphi'_{49})-$$
$$-2(\varphi'_{19}+\varphi'_{20}+\varphi'_{28}+\varphi'_{32}+\varphi'_{43}+\varphi'_{47}+\varphi'_{53}+\varphi'_{54})\}$$

$$\varphi_{T_{19}}=\frac{\sqrt{6}}{12}\{2(\varphi'_{19}+\varphi'_{53})+$$
$$+1(\varphi'_{29}+\varphi'_{33}+\varphi'_{44}+\varphi'_{48})-$$
$$-2(\varphi'_{20}+\varphi'_{54})-$$
$$-1(\varphi'_{30}+\varphi'_{34}+\varphi'_{45}+\varphi'_{49})\}$$

$$\varphi_{T_{20}}=\frac{\sqrt{5}}{60}\{12(\varphi'_{21})+$$
$$+3(\varphi'_{37}+\varphi'_{38}+\varphi'_{39}+\varphi'_{40}+\varphi'_{42}+\varphi'_{43}+\varphi'_{46}+\varphi'_{47})+$$
$$+2(\varphi'_{26}+\varphi'_{29}+\varphi'_{30}+\varphi'_{33}+\varphi'_{34}+\varphi'_{35})-$$
$$-12(\varphi'_{36})-$$
$$-3(\varphi'_{22}+\varphi'_{23}+\varphi'_{24}+\varphi'_{25}+\varphi'_{27}+\varphi'_{28}+\varphi'_{31}+\varphi'_{32})-$$
$$-2(\varphi'_{41}+\varphi'_{44}+\varphi'_{45}+\varphi'_{48}+\varphi'_{49}+\varphi'_{50})\}$$

$$\varphi_{T_{21}}=\frac{\sqrt{2}}{24}\{9(\varphi'_{22})+$$
$$+3(\varphi'_{38}+\varphi'_{39}+\varphi'_{42}+\varphi'_{46})+$$

$$+2(\varphi^1_{30}+\varphi^1_{34}+\varphi^1_{35}+\varphi^1_{41}+\varphi^1_{44}+\varphi^1_{48})+$$
$$+1(\varphi^1_{25}+\varphi^1_{28}+\varphi^1_{32})-$$
$$-9(\varphi^1_{37})-$$
$$-3(\varphi^1_{23}+\varphi^1_{24}+\varphi^1_{27}+\varphi^1_{31})-$$
$$-2(\varphi^1_{26}+\varphi^1_{29}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{49}+\varphi^1_{50})-$$
$$-1(\varphi^1_{40}+\varphi^1_{43}+\varphi^1_{47})\}$$

$$\varphi_{T_{22}}=\frac{1}{6}\{3(\varphi^1_{23})+$$
$$+1(\varphi^1_{29}+\varphi^1_{32}+\varphi^1_{35}+\varphi^1_{40}+\varphi^1_{41}+\varphi^1_{43}+\varphi^1_{44}+\varphi^1_{47}+\varphi^1_{48})-$$
$$-3(\varphi^1_{38})-$$
$$-1(\varphi^1_{25}+\varphi^1_{26}+\varphi^1_{28}+\varphi^1_{29}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{49}+\varphi^1_{50})\}$$

$$\varphi_{T_{23}}=\frac{1}{12}\{6(\varphi^1_{24})+$$
$$+3(\varphi^1_{42}+\varphi^1_{46})+$$
$$+2(\varphi^1_{35}+\varphi^1_{40}+\varphi^1_{41})+$$
$$+1(\varphi^1_{28}+\varphi^1_{29}+\varphi^1_{32}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{49})-$$
$$-6(\varphi^1_{39})-$$
$$-3(\varphi^1_{27}+\varphi^1_{31})-$$
$$-2(\varphi^1_{25}+\varphi^1_{26}+\varphi^1_{50})-$$
$$-1(\varphi^1_{30}+\varphi^1_{34}+\varphi^1_{43}+\varphi^1_{44}+\varphi^1_{47}+\varphi^1_{48})\}$$

$$\varphi_{T_{24}}=\frac{\sqrt{2}}{12}\{4(\varphi^1_{25})$$
$$+2(\varphi^1_{35}+\varphi^1_{41}+\varphi^1_{43}+\varphi^1_{47})+$$
$$+1(\varphi^1_{29}+\varphi^1_{33}+\varphi^1_{45}+\varphi^1_{49})-$$
$$-4(\varphi^1_{40})-$$
$$-2(\varphi^1_{26}+\varphi^1_{28}+\varphi^1_{32}+\varphi^1_{50})-$$
$$-1(\varphi^1_{30}+\varphi^1_{34}+\varphi^1_{44}+\varphi^1_{48})\}$$

$$\varphi_{T_{25}} = \frac{\sqrt{6}}{12}\{2(\varphi'_{26} + \varphi'_{35}) + $$
$$+ 1(\varphi'_{44} + \varphi'_{45} + \varphi'_{48} + \varphi'_{49}) -$$
$$- 2(\varphi'_{41} + \varphi'_{50}) -$$
$$- 1(\varphi'_{29} + \varphi'_{30} + \varphi'_{33} + \varphi'_{34})\}$$

$$\varphi_{T_{26}} = \frac{\sqrt{3}}{12}\{3(\varphi'_{27} + \varphi'_{46}) +$$
$$+ 1(\varphi'_{32} + \varphi'_{33} + \varphi'_{34} + \varphi'_{43} + \varphi'_{44} + \varphi'_{45}) -$$
$$- 3(\varphi'_{31} + \varphi'_{42}) -$$
$$- 1(\varphi'_{28} + \varphi'_{29} + \varphi'_{30} + \varphi'_{47} + \varphi'_{48} + \varphi'_{49})\}$$

$$\varphi_{T_{27}} = \frac{\sqrt{6}}{12}\{2(\varphi'_{28} + \varphi'_{47}) +$$
$$+ 1(\varphi'_{33} + \varphi'_{34} + \varphi'_{44} + \varphi'_{45}) -$$
$$- 2(\varphi'_{32} + \varphi'_{43}) -$$
$$- 1(\varphi'_{29} + \varphi'_{30} + \varphi'_{48} + \varphi'_{49})\}$$

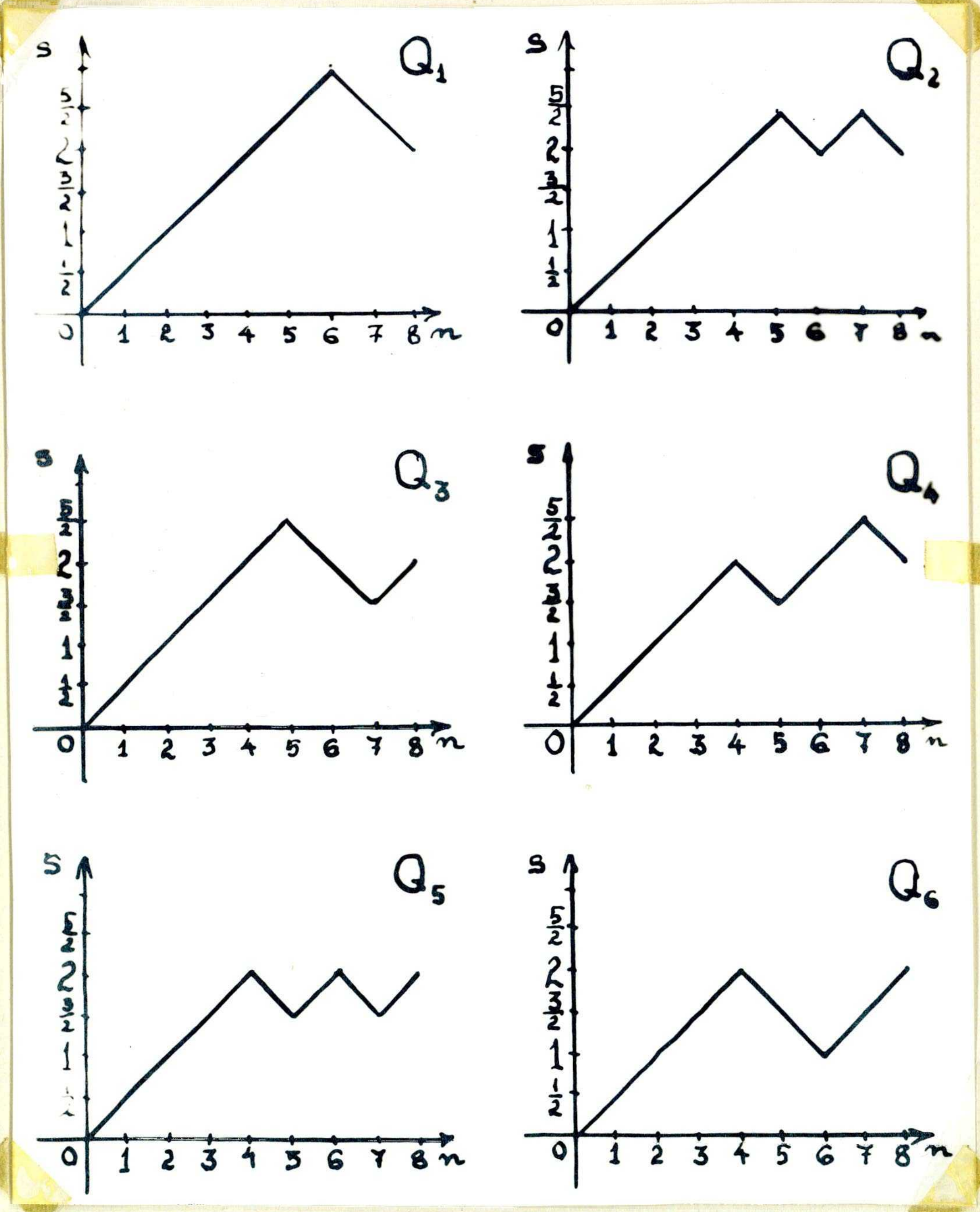
$$\varphi_{T_{28}} = \frac{\sqrt{2}}{4}\{1(\varphi'_{29} + \varphi'_{34} + \varphi'_{45} + \varphi'_{48}) -$$
$$- 1(\varphi'_{30} + \varphi'_{33} + \varphi'_{43} + \varphi'_{49})\}$$

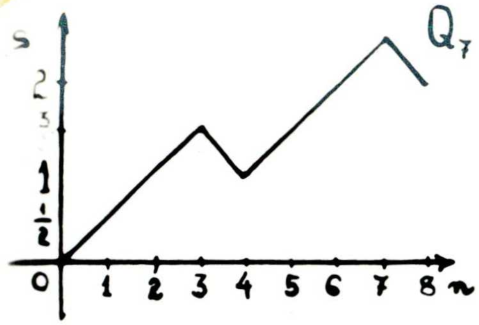
C./ Quintettek

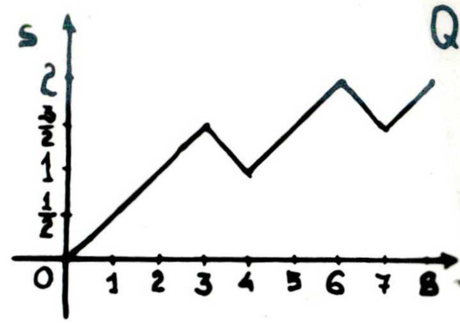
A 2 eredő spinhez tartozó SLATER-determinánsokat a következőképpen jelöljük :

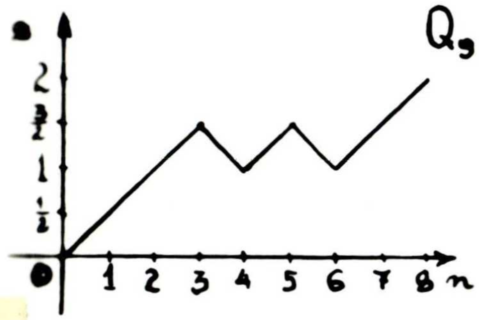
$$\varphi_1^2 = |\alpha\alpha\alpha\alpha\alpha\alpha\beta\beta|$$
$$\varphi_2^2 = |\alpha\alpha\alpha\alpha\alpha\beta\alpha\beta|$$
$$\varphi_3^2 = |\alpha\alpha\alpha\alpha\alpha\beta\beta\alpha|$$
$$\varphi_4^2 = |\alpha\alpha\alpha\alpha\beta\alpha\alpha\beta|$$
$$\varphi_5^2 = |\alpha\alpha\alpha\alpha\beta\alpha\beta\alpha|$$
$$\varphi_6^2 = |\alpha\alpha\alpha\alpha\beta\beta\alpha\alpha|$$
$$\varphi_7^2 = |\alpha\alpha\alpha\beta\alpha\alpha\alpha\beta|$$
$$\varphi_8^2 = |\alpha\alpha\alpha\beta\alpha\alpha\beta\alpha|$$
$$\varphi_9^2 = |\alpha\alpha\alpha\beta\alpha\beta\alpha\alpha|$$
$$\varphi_{10}^2 = |\alpha\alpha\alpha\beta\beta\alpha\alpha\alpha|$$
$$\varphi_{11}^2 = |\alpha\alpha\beta\alpha\alpha\alpha\alpha\beta|$$
$$\varphi_{12}^2 = |\alpha\alpha\beta\alpha\alpha\alpha\beta\alpha|$$
$$\varphi_{13}^2 = |\alpha\alpha\beta\alpha\alpha\beta\alpha\alpha|$$
$$\varphi_{14}^2 = |\alpha\alpha\beta\alpha\beta\alpha\alpha\alpha|$$
$$\varphi_{15}^2 = |\alpha\alpha\beta\beta\alpha\alpha\alpha\alpha|$$
$$\varphi_{16}^2 = |\alpha\beta\alpha\alpha\alpha\alpha\alpha\beta|$$
$$\varphi_{17}^2 = |\alpha\beta\alpha\alpha\alpha\alpha\beta\alpha|$$
$$\varphi_{18}^2 = |\alpha\beta\alpha\alpha\alpha\beta\alpha\alpha|$$
$$\varphi_{19}^2 = |\alpha\beta\alpha\alpha\beta\alpha\alpha\alpha|$$
$$\varphi_{20}^2 = |\alpha\beta\alpha\beta\alpha\alpha\alpha\alpha|$$
$$\varphi_{21}^2 = |\alpha\beta\beta\alpha\alpha\alpha\alpha\alpha|$$
$$\varphi_{22}^2 = |\beta\alpha\alpha\alpha\alpha\alpha\alpha\beta|$$
$$\varphi_{23}^2 = |\beta\alpha\alpha\alpha\alpha\alpha\beta\alpha|$$
$$\varphi_{24}^2 = |\beta\alpha\alpha\alpha\alpha\beta\alpha\alpha|$$
$$\varphi_{25}^2 = |\beta\alpha\alpha\alpha\beta\alpha\alpha\alpha|$$
$$\varphi_{26}^2 = |\beta\alpha\alpha\beta\alpha\alpha\alpha\alpha|$$
$$\varphi_{27}^2 = |\beta\alpha\beta\alpha\alpha\alpha\alpha\alpha|$$
$$\varphi_{28}^2 = |\beta\beta\alpha\alpha\alpha\alpha\alpha\alpha|$$

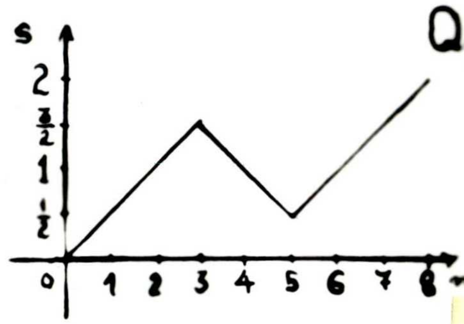
Quintetteket az elágazási diagram szerint 2o féleképpen szerkeszthetünk :

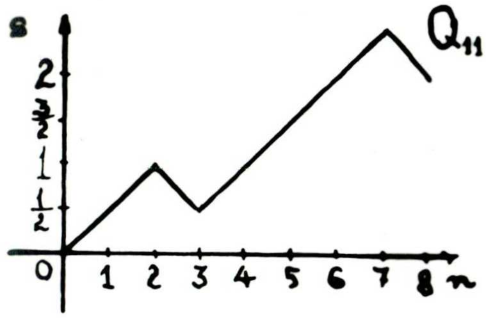


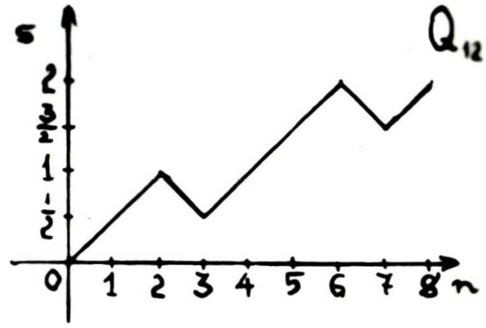

Q7
s
2
1
1/2
0 1 2 3 4 5 6 7 8 n

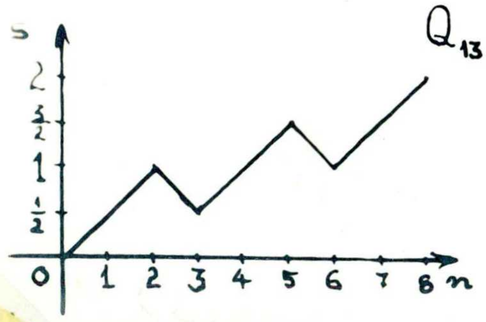

Q8
s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8

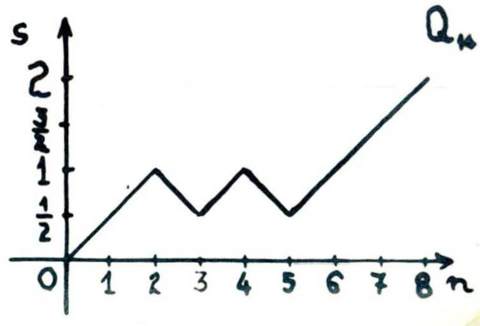

Q9
2
3/2
1
1/2
1 2 3 4 5 6 7 8 n

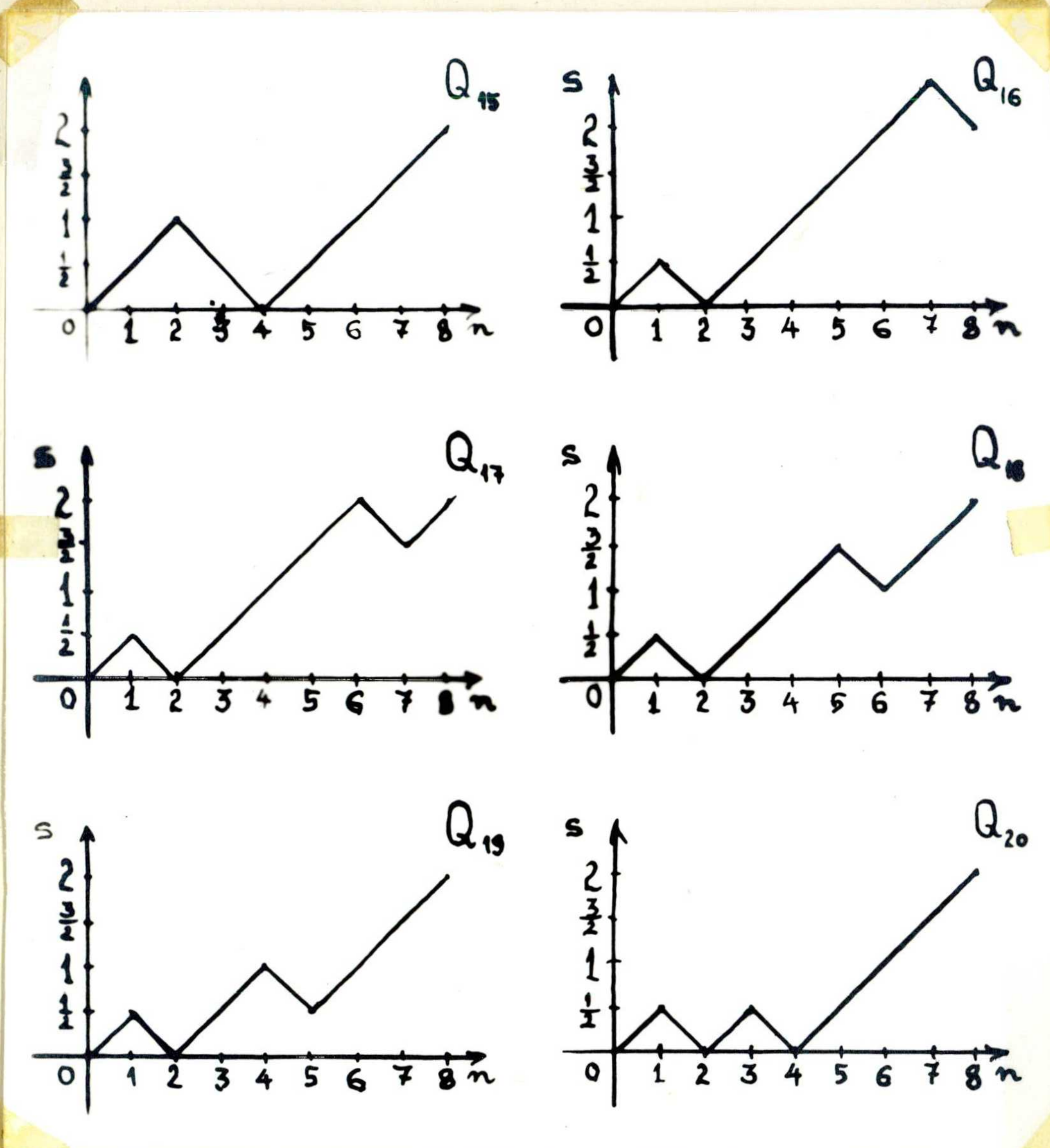

s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8


Q11
s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8 n


Q12
s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8 n


Q13
s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8 n


s
2
3/2
1
1/2
0 1 2 3 4 5 6 7 8 n



A megfelelő sajátfüggvények a következők :

$$\varphi_{Q_1} = \frac{\sqrt{35}}{210}\{30(\varphi_1^2) +$$

$$+ 2(\varphi_6^2 + \varphi_9^2 + \varphi_{10}^2 + \varphi_{13}^2 + \varphi_{14}^2 + \varphi_{15}^2 + \varphi_{18}^2 + \varphi_{19}^2 + \varphi_{20}^2 + \varphi_{21}^2 +$$

$$+ \varphi_{24}^2 + \varphi_{25}^2 + \varphi_{26}^2 + \varphi_{27}^2 + \varphi_{28}^2) -$$

$$-5(\varphi_2^2 + \varphi_3^2 + \varphi_4^2 + \varphi_5^2 + \varphi_7^2 + \varphi_8^2 + \varphi_{11}^2 + \varphi_{12}^2 + \varphi_{16}^2 + \varphi_{17}^2 + \varphi_{22}^2 + \varphi_{23}^2)\}$$

$$\varphi_{Q_2} = \frac{1}{30}\{25(\varphi_2^2) +$$
$$+2(\varphi_{10}^2+\varphi_{14}^2+\varphi_{15}^2+\varphi_{19}^2+\varphi_{20}^2+\varphi_{21}^2+\varphi_{25}^2+\varphi_{26}^2+\varphi_{27}^2+\varphi_{28}^2)+$$
$$+1(\varphi_5^2+\varphi_8^2+\varphi_{12}^2+\varphi_{17}^2+\varphi_{23}^2) -$$
$$-5(\varphi_3^2+\varphi_4^2+\varphi_7^2+\varphi_{11}^2+\varphi_{16}^2+\varphi_{22}^2) -$$
$$-4(\varphi_6^2+\varphi_9^2+\varphi_{13}^2+\varphi_{18}^2+\varphi_{24}^2)\}$$

$$\varphi_{Q_3} = \frac{\sqrt{6}}{30}\{10(\varphi_3^2) +$$
$$+1(\varphi_{10}^2+\varphi_{14}^2+\varphi_{15}^2+\varphi_{19}^2+\varphi_{25}^2+\varphi_{20}^2+\varphi_{21}^2+\varphi_{26}^2+\varphi_{27}^2+\varphi_{28}^2)-$$
$$-2(\varphi_5^2+\varphi_6^2+\varphi_8^2+\varphi_9^2+\varphi_{12}^2+\varphi_{13}^2+\varphi_{17}^2+\varphi_{18}^2+\varphi_{23}^2+\varphi_{24}^2)\}$$

$$\varphi_{Q_4} = \frac{\sqrt{6}}{60}\{20(\varphi_4^2) +$$
$$+2(\varphi_{15}^2+\varphi_{20}^2+\varphi_{21}^2+\varphi_{26}^2+\varphi_{27}^2+\varphi_{28}^2)+$$
$$+1(\varphi_8^2+\varphi_9^2+\varphi_{12}^2+\varphi_{13}^2+\varphi_{17}^2+\varphi_{18}^2+\varphi_{23}^2+\varphi_{24}^2)-$$
$$-5(\varphi_7^2+\varphi_{11}^2+\varphi_{16}^2+\varphi_{22}^2) -$$
$$-4(\varphi_5^2+\varphi_6^2) -$$
$$-3(\varphi_{10}^2+\varphi_{14}^2+\varphi_{19}^2+\varphi_{25}^2)\}$$

$$\varphi_{Q_5} = \frac{1}{20}\{16(\varphi_5^2) +$$
$$+2(\varphi_{15}^2+\varphi_{20}^2+\varphi_{21}^2+\varphi_{26}^2+\varphi_{27}^2+\varphi_{28}^2)+$$
$$+1(\varphi_9^2+\varphi_{13}^2+\varphi_{18}^2+\varphi_{24}^2) -$$
$$-4(\varphi_6^2+\varphi_8^2+\varphi_{12}^2+\varphi_{17}^2+\varphi_{23}^2) -$$
$$-3(\varphi_{10}^2+\varphi_{14}^2+\varphi_{19}^2+\varphi_{25}^2)\}$$

$$\varphi_{Q_6} = \frac{\sqrt{15}}{60}\{12(\varphi_6^2) +$$
$$+2(\varphi_{15}^2+\varphi_{20}^2+\varphi_{21}^2+\varphi_{26}^2+\varphi_{27}^2+\varphi_{28}^2) -$$
$$-3(\varphi_9^2+\varphi_{10}^2+\varphi_{13}^2+\varphi_{14}^2+\varphi_{18}^2+\varphi_{19}^2+\varphi_{24}^2+\varphi_{25}^2)\}$$

$$
\begin{aligned}
\varphi_{Q_7} = \frac{\sqrt{10}}{60}\{ & 15\,(\varphi_7^2) + \\
& + 2\,(\varphi_{21}^2 + \varphi_{27}^2 + \varphi_{28}^2) + \\
& + 1\,(\varphi_{12}^2 + \varphi_{13}^2 + \varphi_{14}^2 + \varphi_{17}^2 + \varphi_{18}^2 + \varphi_{19}^2 + \varphi_{23}^2 + \varphi_{24}^2 + \varphi_{25}^2) - \\
& - 5\,(\varphi_{11}^2 + \varphi_{16}^2 + \varphi_{22}^2) - \\
& - 3\,(\varphi_8^2 + \varphi_9^2 + \varphi_{10}^2) \\
& - 2\,(\varphi_{15}^2 + \varphi_{20}^2 + \varphi_{26}^2)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_8} = \frac{\sqrt{15}}{60}\{ & 12\,(\varphi_8^2) + \\
& + 2\,(\varphi_{21}^2 + \varphi_{27}^2 + \varphi_{28}^2) + \\
& + 1\,(\varphi_{13}^2 + \varphi_{14}^2 + \varphi_{18}^2 + \varphi_{19}^2 + \varphi_{24}^2 + \varphi_{25}^2) - \\
& - 4\,(\varphi_{12}^2 + \varphi_{17}^2 + \varphi_{23}^2) - \\
& - 3\,(\varphi_9^2 + \varphi_{10}^2) - \\
& - 2\,(\varphi_{15}^2 + \varphi_{20}^2 + \varphi_{26}^2)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_9} = \frac{1}{12}\{ & 9\,(\varphi_9^2) + \\
& + 2\,(\varphi_{21}^2 + \varphi_{27}^2 + \varphi_{28}^2) + \\
& + 1\,(\varphi_{14}^2 + \varphi_{19}^2 + \varphi_{25}^2) - \\
& - 3\,(\varphi_{10}^2 + \varphi_{13}^2 + \varphi_{18}^2 + \varphi_{24}^2) - \\
& - 2\,(\varphi_{15}^2 + \varphi_{20}^2 + \varphi_{26}^2)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{10}} = \frac{\sqrt{2}}{6}\{ & 3\,(\varphi_{10}^2) + \\
& + 1\,(\varphi_{21}^2 + \varphi_{27}^2 + \varphi_{28}^2) - \\
& - 1\,(\varphi_{14}^2 + \varphi_{15}^2 + \varphi_{19}^2 + \varphi_{20}^2 + \varphi_{25}^2 + \varphi_{26}^2)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{11}} = \frac{\sqrt{5}}{30}\{ & 10\,(\varphi_{11}^2) + \\
& + 2\,(\varphi_{28}^2) +
\end{aligned}
$$

$$
\begin{aligned}
&+1\left(\varphi_{17}^2+\varphi_{18}^2+\varphi_{19}^2+\varphi_{20}^2+\varphi_{23}^2+\varphi_{24}^2+\varphi_{25}^2+\varphi_{26}^2\right)-\\
&-5\left(\varphi_{16}^2+\varphi_{22}^2\right)-\\
&-2\left(\varphi_{12}^2+\varphi_{13}^2+\varphi_{14}^2+\varphi_{15}^2\right)-\\
&-1\left(\varphi_{21}^2+\varphi_{27}^2\right)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{12}}=\frac{\sqrt{30}}{60}\{&8\left(\varphi_{12}^2\right)+\\
&+2\left(\varphi_{28}^2\right)+\\
&+1\left(\varphi_{18}^2+\varphi_{19}^2+\varphi_{20}^2+\varphi_{24}^2+\varphi_{25}^2+\varphi_{26}^2\right)-\\
&-4\left(\varphi_{17}^2+\varphi_{23}^2\right)-\\
&-2\left(\varphi_{13}^2+\varphi_{14}^2+\varphi_{15}^2\right)-\\
&-1\left(\varphi_{21}^2+\varphi_{27}^2\right)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{13}}=\frac{\sqrt{2}}{12}\{&6\left(\varphi_{13}^2\right)+\\
&+2\left(\varphi_{28}^2\right)+\\
&+1\left(\varphi_{19}^2+\varphi_{20}^2+\varphi_{25}^2+\varphi_{26}^2\right)-\\
&-3\left(\varphi_{18}^2+\varphi_{24}^2\right)-\\
&-2\left(\varphi_{14}^2+\varphi_{15}^2\right)-\\
&-1\left(\varphi_{21}^2+\varphi_{27}^2\right)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{14}}=\frac{1}{6}\{&4\left(\varphi_{14}^2\right)+\\
&+2\left(\varphi_{28}^2\right)+\\
&+1\left(\varphi_{20}^2+\varphi_{26}^2\right)-\\
&-2\left(\varphi_{15}^2+\varphi_{19}^2+\varphi_{25}^2\right)-\\
&-1\left(\varphi_{21}^2+\varphi_{27}^2\right)\}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_{Q_{15}}=\frac{\sqrt{3}}{6}\{&2\left(\varphi_{15}^2+\varphi_{28}^2\right)-\\
&-1\left(\varphi_{20}^2+\varphi_{21}^2+\varphi_{26}^2+\varphi_{27}^2\right)\}
\end{aligned}
$$

$$\varphi_{Q_{16}} = \frac{\sqrt{15}}{30}\{5(\varphi_{16}^2) + $$
$$+ 1(\varphi_{23}^2 + \varphi_{24}^2 + \varphi_{25}^2 + \varphi_{26}^2 + \varphi_{27}^2) -$$
$$- 5(\varphi_{22}^2) -$$
$$- 1(\varphi_{17}^2 + \varphi_{18}^2 + \varphi_{19}^2 + \varphi_{20}^2 + \varphi_{21}^2)\}$$

$$\varphi_{Q_{17}} = \frac{\sqrt{10}}{20}\{4(\varphi_{17}^2) +$$
$$+ 1(\varphi_{24}^2 + \varphi_{25}^2 + \varphi_{26}^2 + \varphi_{27}^2) -$$
$$- 4(\varphi_{23}^2) -$$
$$- 1(\varphi_{18}^2 + \varphi_{19}^2 + \varphi_{20}^2 + \varphi_{21}^2)\}$$

$$\varphi_{Q_{18}} = \frac{\sqrt{6}}{12}\{3(\varphi_{18}^2) +$$
$$+ 1(\varphi_{25}^2 + \varphi_{26}^2 + \varphi_{27}^2) -$$
$$- 3(\varphi_{24}^2) -$$
$$- 1(\varphi_{19}^2 + \varphi_{20}^2 + \varphi_{21}^2)\}$$

$$\varphi_{Q_{19}} = \frac{\sqrt{3}}{6}\{2(\varphi_{19}^2) +$$
$$+ 1(\varphi_{26}^2 + \varphi_{27}^2) - 2(\varphi_{25}^2) -$$
$$- 1(\varphi_{20}^2 + \varphi_{21}^2)\}$$

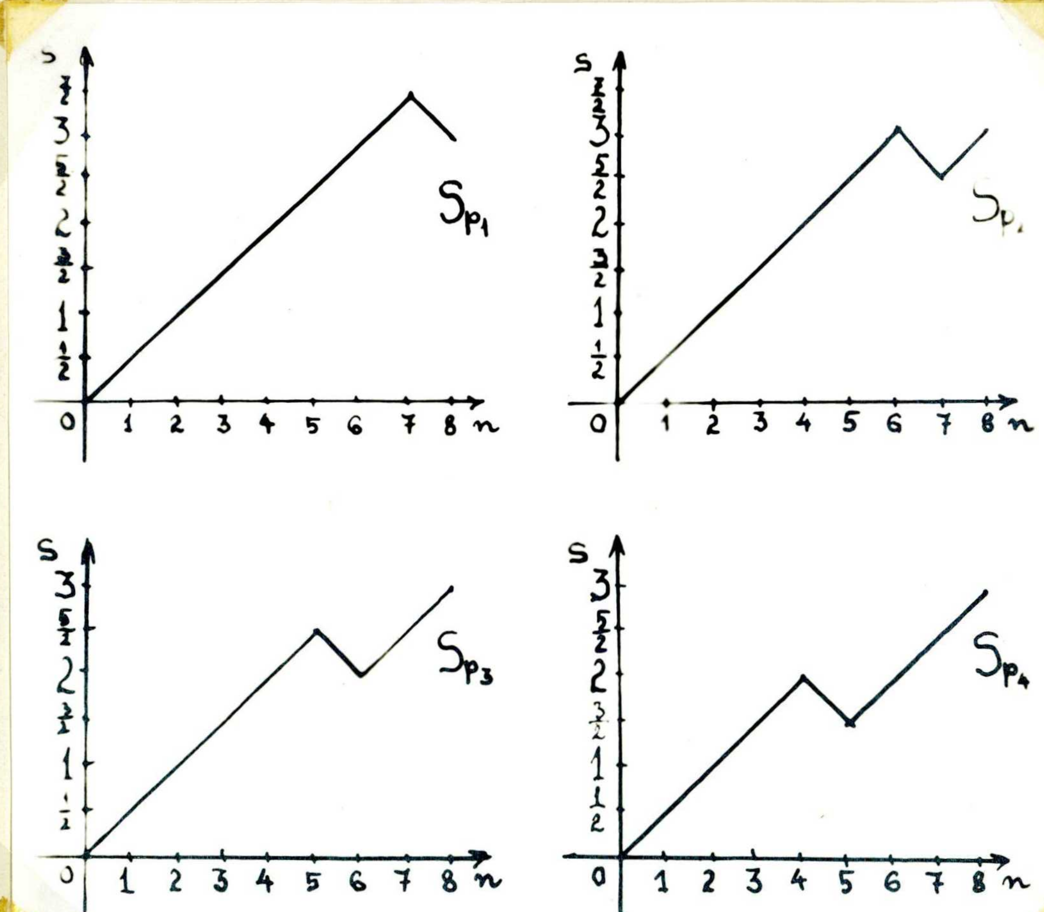
$$\varphi_{Q_{20}} = \frac{1}{2}\{1(\varphi_{20}^2 + \varphi_{27}^2) -$$
$$- 1(\varphi_{21}^2 + \varphi_{26}^2)\}$$

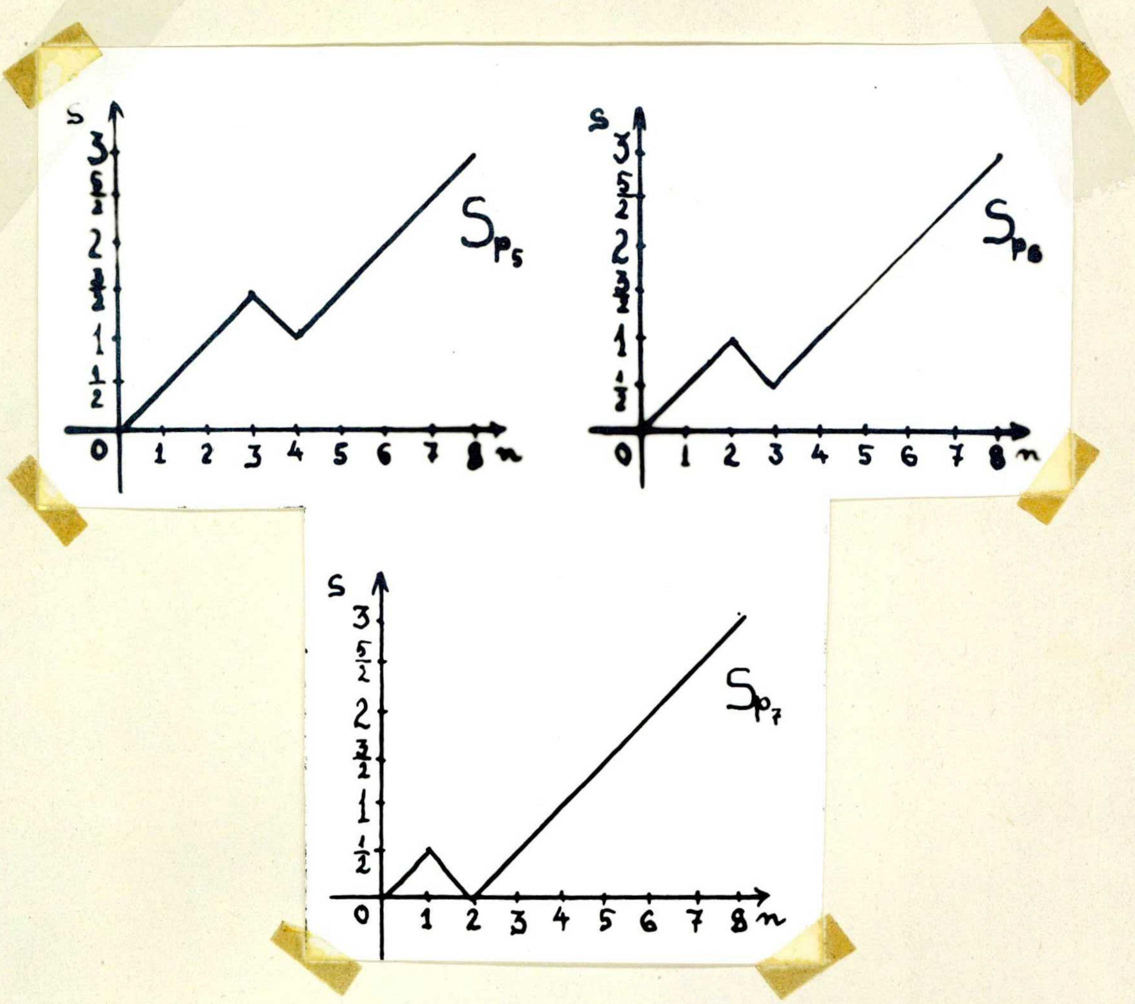
D./ Szeptettek

A 4 eredő spinhez tartozó SLATER-determinánsokat a következőképpen jelöljük :

$$\varphi_1^3 = |\alpha\alpha\alpha\alpha\alpha\alpha\alpha\beta| \qquad \varphi_5^3 = |\alpha\alpha\alpha\beta\alpha\alpha\alpha\alpha|$$
$$\varphi_2^3 = |\alpha\alpha\alpha\alpha\alpha\alpha\beta\alpha| \qquad \varphi_6^3 = |\alpha\alpha\beta\alpha\alpha\alpha\alpha\alpha|$$
$$\varphi_3^3 = |\alpha\alpha\alpha\alpha\alpha\beta\alpha\alpha| \qquad \varphi_7^3 = |\alpha\beta\alpha\alpha\alpha\alpha\alpha\alpha|$$
$$\varphi_4^3 = |\alpha\alpha\alpha\alpha\beta\alpha\alpha\alpha| \qquad \varphi_8^3 = |\beta\alpha\alpha\alpha\alpha\alpha\alpha\alpha|$$

Szeptetteket az elágazási diagram szerint hétféleképpen szerkeszthetünk :





A megfelelő sajátfüggvények a következők :

$$\varphi_{S_{p1}} = \frac{\sqrt{14}}{28}\left\{7\left(\varphi_1^3\right) - \right.$$
$$\left. - 1\left(\varphi_2^3 + \varphi_3^3 + \varphi_4^3 + \varphi_5^3 + \varphi_6^3 + \varphi_7^3 + \varphi_8^3\right)\right\}$$

$$\varphi_{S_{p2}} = \frac{\sqrt{42}}{42}\left\{6\left(\varphi_2^3\right) - \right.$$
$$\left. - 1\left(\varphi_3^3 + \varphi_4^3 + \varphi_5^3 + \varphi_6^3 + \varphi_7^3 + \varphi_8^3\right)\right\}$$

$$\varphi_{Sp3} = \frac{\sqrt{30}}{30}\{5(\varphi_3^3) - 1(\varphi_4^3 + \varphi_5^3 + \varphi_6^3 + \varphi_7^3 + \varphi_8^3)\}$$

$$\varphi_{Sp4} = \frac{\sqrt{5}}{10}\{4(\varphi_4^3) - 1(\varphi_5^3 + \varphi_6^3 + \varphi_7^3 + \varphi_8^3)\}$$

$$\varphi_{Sp5} = \frac{\sqrt{3}}{6}\{3(\varphi_5^3) - 1(\varphi_6^3 + \varphi_7^3 + \varphi_8^3)\}$$

$$\varphi_{Sp6} = \frac{\sqrt{6}}{6}\{2(\varphi_6^3) - 1(\varphi_7^3 + \varphi_8^3)\}$$

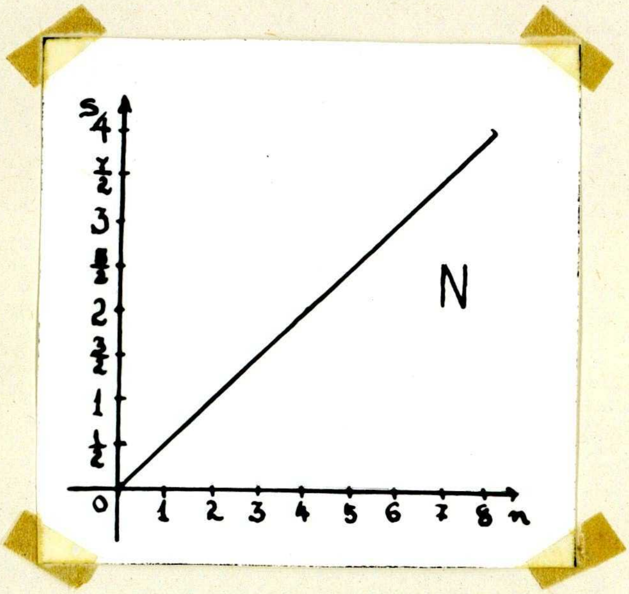
$$\varphi_{Sp7} = \frac{\sqrt{2}}{2}\{\varphi_7^3 - \varphi_8^3\}$$

E./ Nonett

Az 5 eredő spinhez tartozó SLATER-determinánst a következőképpen jelöljük :

$$\varphi_1^4 = |\alpha\alpha\alpha\alpha\alpha\alpha\alpha\alpha|$$

Nonettet az elágazási diagram szerint egyféleképpen szerkeszthetünk :



A megfelelő sajátfüggvény a következő :

$$\varphi_N = \varphi_1^4$$

Irodalom

[1] BERENCZ, F. : Proc. Phys. Soc. 71. 145. 1958.

[2] CORSON, E. M. : Perturbation methods in the quantum mechanics of n-elektron system. Blackie, London and Glasgow 1951.

[3] EYRING, H. - WALTER, J. - KIMBALL, G. E. : Quantum Chemistry, Wiley, New York 1949.

[4] VAN DER WAERDEN, B. L. : Die Gruppentheoretische Methode in der Quantenmechanik. Springer. Berlin 1932.