2/a. 8 different det's w/ 1 e^- in each orbital:

$|a\,b\,c|$ all spin up

$|\bar{a}\,bc|$, $|a\bar{b}\,c|$, $|ab\bar{c}|$ 2 spin-up, 1 spin down

$|\bar{a}\bar{b}c|$, $|a\bar{b}\bar{c}|$, $|\bar{a}b\bar{c}|$ 2 spin down, 1 spin up

$|\bar{a}\bar{b}\bar{c}|$ all spin down.

b. Let $|abc\rangle = \phi_a(1)\alpha(1)\,\phi_b(2)\alpha(2)\,\phi_c(3)\alpha(3)$ all spin up.

Then $\Psi(3/2) = \frac{1}{\sqrt{3!}}(abc - bac + bca - acb + cab - cba)\,\alpha(1)\alpha(2)\alpha(3)$

($N! = 3! = 6$ terms)

$$\langle \Psi_{3/2}|H|\Psi_{3/2}\rangle = \langle A(\phi_a\phi_b\phi_c)|\mathcal{H}|A(\phi_a\phi_b\phi_c)\rangle$$

$$= \langle abc|\mathcal{H}|(abc - bac + bca - acb + cab - cba)\rangle$$

$$= \sum_{i=1}^{3}\left[\langle abc|h(i)|abc\rangle - \langle abc|h(i)|bac\rangle + \cdots\right.$$

$$+ e^2 \underbrace{\sum_{i<j}}_{3\,\text{prs}} \sum_j \langle abc|r_{ij}|abc\rangle - \langle abc|r_{ij}|bac\rangle + \cdots$$

for 1 e^- operator, $h(i)$, MATRIX ELEMENTS:

$$\sum_{i=1}^{3}\langle abc|h(i)|abc\rangle = \langle a|h|a\rangle + \langle b|h|b\rangle + \langle c|h|c\rangle$$

$$= W_a + W_b + W_c$$

$$\sum_{i=1}^{3} \langle abc | h(i) | bac \rangle = \cancel{\langle abc | h(1) | bac \rangle} + \cancel{\langle abc | h(2) | bac \rangle} + \cancel{\langle abc | h(3) | bac \rangle}$$

integral over $\vec{r}_2$ gives 0 — integral over $\vec{r}_1$ gives zero — integral over $\vec{r}_1$ gives zero

2.

The rest of the matrix elements also give $\underline{\underline{0}}$

For $2e^-$ operator:

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | abc \rangle = \langle ab | 1/r_{12} | ab \rangle + \langle ac | 1/r_{13} | ac \rangle + \langle bc | 1/r_{23} | bc \rangle$$

$$= J_{ab} + J_{ac} + J_{bc}.$$

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | bac \rangle = \langle ab | 1/r_{12} | ba \rangle + \cancel{\langle ac | 1/r_{13} | bc \rangle} + \cancel{\langle bc | 1/r_{23} | ac \rangle}$$

integral over $\vec{r}_2$ gives 0 — integral over $\vec{r}_1 = 0$

$$= K_{ab}$$

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | bca \rangle = 0$$

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | acb \rangle = K_{bc}$$

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | cab \rangle = 0$$

$$e^2 \sum_{i<j}^{3} \langle abc | 1/r_{ij} | cba \rangle = K_{ac}$$

So: $\langle \Psi_{3/2} | H | \Psi_{3/2} \rangle = W_a + W_b + W_c + J_{ab} + J_{ac} + J_{bc} - K_{ab} - K_{ac} - K_{bc}.$

c) For example, $|\bar{a}bc|$ has $M_s = \frac{1}{2}$

$$E = W_a + W_b + W_c + J_{ab} + J_{bc} + J_{ac} - K_{bc}$$

3.

d) Each Slater determinant is an eigenfunction of S_z so each must have a well defined $M_s = m_{s_1} + m_{s_2} + m_{s_3}$. They can be denoted by $|\alpha M_s\rangle$ (α is some set of q.n's)

Start w/ $[H, S_z] = 0$

$$\Downarrow$$

$$S_z H = H S_z$$

Left multiply by $\langle M_s'|$ & right multiply by $|M_s\rangle$ to get:

$$\langle M_s'| S_z H |M_s\rangle = \langle M_s'| H S_z |M_s\rangle$$

S_z is Hermitian $\Rightarrow$ $S_z^+ = S_z$ $\therefore$ we can let it left operate on $\langle M_s'|$ & right operate on $|M_s\rangle$

$$\langle M_s'| S_z = M_s'\hbar \langle M_s'|$$
$$S_z |M_s\rangle = M_s\hbar |M_s\rangle$$

So $M_s'\hbar \langle M_s'|H|M_s\rangle = M_s\hbar \langle M_s'|H|M_s\rangle$

$$(M_s' - M_s)\hbar \langle M_s'|H|M_s\rangle = 0$$

if $M_s' \neq M_s$ then $\langle M_s'|H|M_s\rangle = 0$

so H cannot couple determinants with different M_s.

So the only non-zero matrix elements occur for determinants with equal M_s.