Spin Hamiltonian Matrices
Axial Systems

***S* = 1/2**

$S = 1/2$	$+1/2$	$-1/2$
$+1/2$	$g_z \beta H_z/2$	$g_x \beta H_x/2$
$-1/2$	$g_x \beta H_x/2$	$-g_z \beta H_z/2$

eigenvalues:

for $H_x = 0$: $\pm g_z \beta H_z$;

for $H_z = 0$: $\pm g_x \beta H_x$.

***S* = 1**

diagonal: $D\boldsymbol{S}_z^2 + g_z\beta H \cong \boldsymbol{S}_z = DM_S^2 + g_z\beta H_z M_S$
off-diagonal: $g_x\beta H \cong \boldsymbol{S}_x = g_x\beta H_x\ (1/2)(\boldsymbol{S}_+ + \boldsymbol{S}_-)$; $\boldsymbol{S}_\pm = \{S(S+1) - M_S(M_S \pm 1)\}^{1/2} = 2^{1/2}$ for $S = 1$.

$S = 1$	+1	0	-1
+1	$D + g_z\beta H_z$	$g_x\beta H_x/2^{1/2}$	0
0	$g_x\beta H_x/2^{1/2}$	0	$g_x\beta H_x/2^{1/2}$
-1	0	$g_x\beta H_x/2^{1/2}$	$D - g_z\beta H_z$

Eigenvalues ($E_{1,2,3}$, ascending value):

For $H_{x,\,z} = 0$: 0, D (2).

For $H_x = 0$: 0, $D \pm g_z\beta H_z$; assuming $D > 0$ and $D > g_z\beta H_z$,
$E_{1z} = 0$,
$E_{2z} = D - g_z\beta H_z$,
$E_{3z} = D + g_z\beta H_z$.

Thus,
$g_z = (E_{3z} - E_{2z})/(2\beta H_z)$ and
$D = (E_{3z} + E_{2z})/2$

For $H_z = 0$: D, $[D \pm \{D^2 + (2g_x\beta H_x)^2\}^{1/2}]/2$; assuming $D > 0$ and $D > g_x\beta H_x$,
$E_{1x} = [D - \{D^2 + (2g_x\beta H_x)^2\}^{1/2}]/2$,
$E_{2x} = D$,
$E_{3x} = [D + \{D^2 + (2g_x\beta H_x)^2\}^{1/2}]/2$.

Thus,
$g_x = [(E_{3x} - E_{1x})^2 - D^2]^{1/2}/(2\beta H_x)$.

***S* = 3/2**

$S = 3/2$	+3/2	+1/2	-1/2	-3/2
+3/2	$(9/4)D + g_z\beta H_z(3/2)$	$g_x\beta H_x(3^{1/2}/2)$	0	0
+1/2	$g_x\beta H_x(3^{1/2}/2)$	$(1/4)D + g_z\beta H_z/2$	$g_x\beta H_x$	0
-1/2	0	$g_x\beta H_x$	$(1/4)D - g_z\beta H_z/2$	$g_x\beta H_x(3^{1/2}/2)$
-3/2	0	0	$g_x\beta H_x(3^{1/2}/2)$	$(9/4)D - g_z\beta H_z(3/2)$

Eigenvalues ($E_{1,2,3,4}$, ascending value):

For $H_{x,\,z} = 0$: 0 (2), $2D$ (2) {ground state / 0}.

For $H_x = 0$: $(9/4)D \pm (3/2)g_z\beta H_z$, $(1/4)D \pm (1/2)g_z\beta H_z$; assuming $D > 0$ and $D > g_z\beta H_z$,
$E_{1z} = (1/4)D - (1/2)g_z\beta H_z$,
$E_{2z} = (1/4)D + (1/2)g_z\beta H_z$,
$E_{3z} = (9/4)D - (3/2)g_z\beta H_z$,
$E_{4z} = (9/4)D + (3/2)g_z\beta H_z$,

thus,
$g_z = (E_{2z} - E_{1z})/(\beta H_z)$ and
$g_z = (E_{4z} - E_{3z})/(3\beta H_x)$ and
$D = 2(E_{2z} + E_{1z})$ and
$D = (2/9)(E_{4z} + E_{3z})$.

For $H_z = 0$: $(1/4)[5D \pm 2g_x\beta H_x \pm 4\{D^2 \text{ K } D\, g_x\beta H_x + (g_x\beta H_x)^2\}^{1/2}]$; assuming $D > 0$ and $D > g_x\beta H_x$,
$E_{1x} = (1/4)[5D - 2g_x\beta H_x - 4\{D^2 + D\, g_x\beta H_x + (g_x\beta H_x)^2\}^{1/2}]$,
$E_{2x} = (1/4)[5D + 2g_x\beta H_x - 4\{D^2 - D\, g_x\beta H_x + (g_x\beta H_x)^2\}^{1/2}]$,
$E_{3x} = (1/4)[5D - 2g_x\beta H_x + 4\{D^2 + D\, g_x\beta H_x + (g_x\beta H_x)^2\}^{1/2}]$,
$E_{4x} = (1/4)[5D + 2g_x\beta H_x + 4\{D^2 - D\, g_x\beta H_x + (g_x\beta H_x)^2\}^{1/2}]$,

thus,
$g_x = [(E_{4x} + E_{2x}) - (5/2)D]/(\beta H_x)$ and
$g_x = -[(E_{3x} + E_{1x}) - (5/2)D]/(\beta H_x)$.

***S* = 2**

$S = 2$	+2	+1	0	-1	-2
+2	$4D + 2g_z\beta H_z$	$g_x\beta H_x$	0	0	0
+1	$g_x\beta H_x$	$D + g_z\beta H_z$	$g_x\beta H_x(3/2)^{1/2}$	0	0
0	0	$g_x\beta H_x(3/2)^{1/2}$	0	$g_x\beta H_x(3/2)^{1/2}$	0
-1	0	0	$g_x\beta H_x(3/2)^{1/2}$	$D - g_z\beta H_z$	$g_x\beta H_x$
-2	0	0	0	$g_x\beta H_x$	$4D - 2g_z\beta H_z$

Eigenvalues ($E_{1,2,3,4,5}$, ascending value):

For $H_{x,\,z} = 0$: 0, D (2), $4D$ (2).

For $H_x = 0$: 0, $D \pm g_z\beta H_z$, $4D \pm 2\ g_z\beta H_z/2$; assuming $|D| > g_z\beta H_z$ and $D > 0$,
$E_{1z} = 0$,
$E_{2z} = D - g_z\beta H_z$,
$E_{3z} = D + g_z\beta H_z$,
$E_{4z} = 4D - 2\ g_z\beta H_z$,
$E_{5z} = 4D + 2\ g_z\beta H_z$.

thus,
$g_z = (E_{3z} - E_{2z})/(2\beta H_z)$ and $g_z = (E_{5z} - E_{4z})/(4\beta H_z)$ and
$D = (E_{3z} + E_{2z})/2$ and $D = (E_{5z} + E_{4z})/8$.
(For $D < 0$, the eigenvalue order is reversed so $E_{1z} \rightarrow E_{5z}$, etc., so
$g_z = (E_{3z} - E_{4z})/(2\beta H_z)$ and $g_z = (E_{1z} - E_{2z})/(4\beta H_z)$ and
$D = (E_{3z} + E_{4z})/2$ and $D = (E_{1z} + E_{2z})/8$).

For $H_z = 0$: $(1/2)[5D \pm \{(3D)^2 + (2\ g_x\beta H_x)^2\}^{1/2}]$, plus the three roots of a cubic equation; assuming $|D| > g_x\beta H_x$,

$E_{1x} = (1/3)[5D - \{(1 + 3^{1/2}i)\mathrm{A} + (1 - 3^{1/2}i)\mathrm{B}^2\}/(2\mathrm{B})] \rightarrow 0\ (-\ \varepsilon)$ as $H_x \rightarrow 0$, (root #4)
$E_{2x} = (1/2)[5D - \{(3D)^2 + (2\ g_x\beta H_x)^2\}^{1/2}] \rightarrow D\ (-\ \varepsilon)$ as $H_x \rightarrow 0$, (root #1)
$E_{3x} = (1/3)[5D - \{(1 - 3^{1/2}i)\mathrm{A} + (1 + 3^{1/2}i)\mathrm{B}^2\}/(2\mathrm{B})] \rightarrow D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$, (root #5)
$E_{4x} = (1/2)[5D + \{(3D)^2 + (2\ g_x\beta H_x)^2\}^{1/2}] \rightarrow 4D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$, (root #2)
$E_{5x} = (1/3)[5D + \{\mathrm{A} + \mathrm{B}^2\}/\mathrm{B}] \rightarrow 4D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$ (E_{4x} . E_{5x}); (root #3)

where,
A = $13D^2 + 12(g_x\beta H_x)^2$
B = $[35D^3 - 72D(g_x\beta H_x)^2 + 6\ 3^{1/2} i\{9D^6 - 103D^4(g_x\beta H_x)^2 + 4D^2(g_x\beta H_x)^4 + 16(g_x\beta H_x)^6\}^{1/2}]^{1/3}$

thus for both $D > 0$ and $D < 0$,
$g_x = [(E_{4x} - E_{2x})^2 - (3D)^2]^{1/2}/(2\beta H_x)$.

***S* = 5/2**

S = 5/2	+5/2	+3/2	+1/2	-1/2	-3/2	-5/2
+5/2	$(25/4)D + g_z\beta H_z(5/2)$	$g_x\beta H_x(5^{1/2}/2)$	0	0	0	0
+3/2	$g_x\beta H_x(5^{1/2}/2)$	$(9/4)D + g_z\beta H_z(3/2)$	$g_x\beta H_x(2^{1/2})$	0	0	0
+1/2	0	$g_x\beta H_x(2^{1/2})$	$(1/4)D + g_z\beta H_z/2$	$g_x\beta H_x(3/2)$	0	0
-1/2	0	0	$g_x\beta H_x(3/2)$	$(1/4)D - g_z\beta H_z/2$	$g_x\beta H_x(2^{1/2})$	0
-3/2	0	0	0	$g_x\beta H_x(2^{1/2})$	$(9/4)D - g_z\beta H_z(3/2)$	$g_x\beta H_x(5^{1/2}/2)$
-5/2	0	0	0	0	$g_x\beta H_x(5^{1/2}/2)$	$(25/4)D - g_z\beta H_z(5/2)$

Eigenvalues ($E_{1,2,3,4,5,6}$, ascending value):

For $H_{x,\,z} = 0$: 0 (2), $2D$ (2), $6D$ (2) {ground state / 0}.

For $H_x = 0$: $(25/4)D \pm g_z\beta H_z(5/2)$, $(9/4)D \pm g_z\beta H_z(3/2)$, $(1/4)D \pm g_z\beta H_z/2$, assuming $D > 0$ and $D > g_z\beta H_z$,

$E_{1z} = (1/4)D - (1/2)g_z\beta H_z$,
$E_{2z} = (1/4)D + (1/2)g_z\beta H_z$,
$E_{3z} = (9/4)D - (3/2)g_z\beta H_z$,
$E_{4z} = (9/4)D + (3/2)g_z\beta H_z$,
$E_{5z} = (25/4)D - (5/2)g_z\beta H_z$,
$E_{6z} = (25/4)D + (5/2)g_z\beta H_z$,

thus,
$g_z = (E_{2z} - E_{1z})/(\beta H_z)$, $g_z = (E_{4z} - E_{3z})/(3\beta H_x)$, and
$g_z = (E_{6z} - E_{5z})/(5\beta H_x)$;
and $D = 2(E_{2z} + E_{1z})$, $D = (2/9)(E_{4z} + E_{3z})$, and
$D = (2/25)(E_{6z} + E_{5z})$.

For $H_z = 0$:
$E_{1x} = (1/12)[35D - 6\, g_z\beta H_z - \{4(1 + 3^{1/2}i)\mathrm{A} + 4(1 - 3^{1/2}i)\mathrm{C}^2\}/\mathrm{C}] \rightarrow (1/4)D\ (-\ \varepsilon)$ as $H_x \rightarrow 0$,(root #5)
$E_{2x} = (1/12)[35D + 6\, g_z\beta H_z - \{4(1 + 3^{1/2}i)\mathrm{B} + 4(1 - 3^{1/2}i)\mathrm{D}^2\}/\mathrm{D}] \rightarrow (1/4)D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$,(root #2)
$E_{3x} = (1/12)[35D - 6\, g_z\beta H_z - \{4(1 - 3^{1/2}i)\mathrm{A} + 4(1 + 3^{1/2}i)\mathrm{C}^2\}/\mathrm{C}] \rightarrow (9/4)D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$,(root #6)
$E_{4x} = (1/12)[35D + 6\, g_z\beta H_z - \{4(1 - 3^{1/2}i)\mathrm{B} + 4(1 + 3^{1/2}i)\mathrm{D}^2\}/\mathrm{D}] \rightarrow (9/4)D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$,(root #3)
$E_{5x} = (1/12)[35D - 6\, g_z\beta H_z + \{8\mathrm{A} + 8\mathrm{C}^2\}/\mathrm{C}] \rightarrow (25/4)D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$, (root #4)
$E_{6x} = (1/12)[35D + 6\, g_z\beta H_z + \{8\mathrm{B} + 8\mathrm{D}^2\}/\mathrm{D}] \rightarrow (25/4)D\ (+\ \varepsilon)$ as $H_x \rightarrow 0$, ($E_{5x} = E_{6x}$); (root #1)
where,
$\mathrm{A} = 2^{2/3}\{7D^2 + 3D(g_x\beta H_x)^2 + 3(g_x\beta H_x)^2\}$
$\mathrm{B} = 2^{2/3}\{7D^2 - 3D(g_x\beta H_x)^2 + 3(g_x\beta H_x)^2\}$
$\mathrm{C} = [40D^3 - 9D^2(g_x\beta H_x) - 36D(g_x\beta H_x)^2 +$
$3\ 3^{1/2}i\{144D^6 + 288D^5(g_x\beta H_x) + 477D^4(g_x\beta H_x)^2 + 216D^3(g_x\beta H_x)^3 + 112D^2(g_x\beta H_x)^4$
$+ 48D(g_x\beta H_x)^5 + 16(g_x\beta H_x)^6\}^{1/2}]^{1/3}$
$\mathrm{D} = [40D^3 + 9D^2(g_x\beta H_x) - 36D(g_x\beta H_x)^2 +$
$3\ 3^{1/2}i\{144D^6 - 288D^5(g_x\beta H_x) + 477D^4(g_x\beta H_x)^2 - 216D^3(g_x\beta H_x)^3 + 112D^2(g_x\beta H_x)^4$
$- 48D(g_x\beta H_x)^5 + 16(g_x\beta H_x)^6\}^{1/2}]^{1/3}$
thus,
$g_x = -[2(E_{1x} + E_{3x} + E_{5x}) - (35/2)D]/(3\beta H_x)$ and
$g_x = [2(E_{2x} + E_{4x} + E_{6x}) - (35/2)D]/(3\beta H_x)$.

Spin Hamiltonian Matrices
Rhombic Systems

diagonal: $B_2^0\ O_2^0 + g_z\beta H\cong\boldsymbol{S}_z$, where $D/3 = B_2^0$;
off-diagonal: $g_x\beta H\cong\boldsymbol{S}_x + g_y\beta H\cong\boldsymbol{S}_y = g_x\beta H_x\ (1/2)(\boldsymbol{S}_+ + \boldsymbol{S}_-) + g_y\beta H_y\ (-i/2)(\boldsymbol{S}_+ - \boldsymbol{S}_-)$;
off-off-diagonal: $B_2^2\ O_2^2$, where $E = B_2^2$.

***S* = 1**

$S = 1$	+1	0	-1
+1	$(1/3)D + g_z\beta H_z$	$(1/2^{1/2})[g_x\beta H_x - i\ g_y\beta H_y]$	E
0	$(1/2^{1/2})[g_x\beta H_x + i\ g_y\beta H_y]$	$(-2/3)D$	$(1/2^{1/2})[g_x\beta H_x - i\ g_y\beta H_y]$
-1	E	$(1/2^{1/2})[g_x\beta H_x + i\ g_y\beta H_y]$	$(1/3)D - g_z\beta H_z$

Eigenvalues ($E_{1,2,3}$, ascending value), assuming $D, E > 0$:

For $H_{x,y,z} = 0$:
$E_1 = (-2/3)D$,
$E_2 = D/3 - E$,
$E_3 = D/3 + E$.
Thus,
$D = \{(E_3 + E_2)/2 - E_1\}$, and $E = (E_3 - E_2)/2$.

For $H_{x,y} = 0$ ($H_z \neq 0$):
$E_{1z} = (-2/3)D$,
$E_{2z} = D/3 - \{E^2 + (g_z\beta H_z)^2\}^{1/2}$,
$E_{3z} = D/3 + \{E^2 + (g_z\beta H_z)^2\}^{1/2}$.
Thus,
$g_z = \{(E_{3z} - E_{2z})^2 - (2E)^2\}^{1/2}/(2\beta H_z)$.

For $H_{y,z} = 0$ ($H_x \neq 0$):
$E_{1x} = (1/2)[-D/3 + E - \{(D + E)^2 + (2\ g_x\beta H_x)^2\}^{1/2}] \rightarrow (-2/3)D\ (-\ \varepsilon)$ as $E, H_x \rightarrow 0$; (root #2)
$E_{2x} = \{D/3 - E\} \rightarrow D/3$ as $E \rightarrow 0$; (root #1)
$E_{3x} = (1/2)[-D/3 + E + \{(D + E)^2 + (2\ g_x\beta H_x)^2\}^{1/2}] \rightarrow D/3\ (+\ \varepsilon)$ as $E, H_x \rightarrow 0$. (root #3)
Thus,
$g_x = \{(E_{3x} - E_{1x})^2 - (D + E)^2\}^{1/2}/(2\beta H_x)$.

For $H_{x,z} = 0$ ($H_y \neq 0$):
$E_{1y} = (1/2)[-D/3 + E - \{(D - E)^2 + (2\, g_y \beta H_y)^2\}^{1/2}] \rightarrow (-2/3)D\ (-\ \varepsilon)$ as $E, H_y \rightarrow 0$; (root #2)
$E_{2y} = \{D/3 - E\} \rightarrow D/3$ as $E \rightarrow 0$; (root #1)
$E_{3y} = (1/2)[-D/3 + E + \{(D - E)^2 + (2\, g_y \beta H_y)^2\}^{1/2}] \rightarrow D/3\ (+\ \varepsilon)$ as $E, H_y \rightarrow 0$. (root #3)
Thus,
$g_y = \{(E_{3y} - E_{1y})^2 - (D - E)^2\}^{1/2}/(2\beta H_y)$.

***S* = 3/2**

$S = 3/2$	+3/2	+1/2	-1/2	-3/2
+3/2	$D + (3/2)\, g_z\beta H_z$	$(3^{1/2}/2)$ $[g_x\beta H_x - i\, g_y\beta H_y]$	$3^{1/2}E$	0
+1/2	$(3^{1/2}/2)$ $[g_x\beta H_x + i\, g_y\beta H_y]$	$-D + (1/2)g_z\beta H_z$	$g_x\beta H_x - i\, g_y\beta H_y$	$3^{1/2}E$
-1/2	$3^{1/2}E$	$g_x\beta H_x + i\, g_y\beta H_y$	$-D - (1/2)g_z\beta H_z$	$(3^{1/2}/2)$ $[g_x\beta H_x - i\, g_y\beta H_y]$
-3/2	0	$3^{1/2}E$	$(3^{1/2}/2)$ $[g_x\beta H_x + i\, g_y\beta H_y]$	$D - (3/2)\, g_z\beta H_z$

Eigenvalues ($E_{1,2,3,4}$, ascending value):

For $H_{x,\,y,\,z} = 0$:
$E_{1,2} = -\{D^2 + 3E^2\}^{1/2}$,
$E_{3,4} = \{D^2 + 3E^2\}^{1/2}$.

For $H_{x,\,y} = 0$ ($H_z \neq 0$), assuming $D > 0$ and $D > g_z\beta H_z$:
$E_{1z} = (1/2)g_z\beta H_z - \{(D + g_z\beta H_z)^2 + 3E^2\}^{1/2} \rightarrow \{-D - (1/2)g_z\beta H_z\}$ as $E \rightarrow 0$; (root #3)
$E_{2z} = -(1/2)g_z\beta H_z - \{(D - g_z\beta H_z)^2 + 3E^2\}^{1/2} \rightarrow \{-D + (1/2)g_z\beta H_z\}$ as $E \rightarrow 0$; (root #1)
$E_{3z} = -(1/2)g_z\beta H_z + \{(D - g_z\beta H_z)^2 + 3E^2\}^{1/2} \rightarrow \{D - (3/2)g_z\beta H_z\}$ as $E \rightarrow 0$; (root #2)
$E_{4z} = (1/2)g_z\beta H_z + \{(D + g_z\beta H_z)^2 + 3E^2\}^{1/2} \rightarrow \{D + (3/2)g_z\beta H_z\}$ as $E \rightarrow 0$; (root #4)

Thus,
$g_z = -(E_{2z} + E_{3z})/(\beta H_z)$ and $g_z = (E_{1z} + E_{4z})/(\beta H_z)$.

For $H_{y,\,z} = 0$ ($H_x \neq 0$), assuming $D > 0$ and $D > g_x\beta H_x$:
$E_{1x} = -(1/2)g_x\beta H_x - \{D^2 + (g_x\beta H_x)^2 + 3E^2 + D(g_x\beta H_x) - 3E(g_x\beta H_x)\}^{1/2} \rightarrow -D$ as $H_x, E \rightarrow 0$; (root #1)
$E_{2x} = (1/2)g_x\beta H_x - \{D^2 + (g_x\beta H_x)^2 + 3E^2 - D(g_x\beta H_x) + 3E(g_x\beta H_x)\}^{1/2} \rightarrow -D$ as $H_x, E \rightarrow 0$; (root #3)
$E_{3x} = -(1/2)g_x\beta H_x + \{D^2 + (g_x\beta H_x)^2 + 3E^2 + D(g_x\beta H_x) - 3E(g_x\beta H_x)\}^{1/2} \rightarrow D$ as $H_x, E \rightarrow 0$; (root #2)
$E_{4x} = (1/2)g_x\beta H_x + \{D^2 + (g_x\beta H_x)^2 + 3E^2 - D(g_x\beta H_x) + 3E(g_x\beta H_x)\}^{1/2} \rightarrow D$ as $H_x, E \rightarrow 0$; (root #4)

Thus,
$g_x = -(E_{1x} + E_{3x})/(\beta H_x)$ and $g_x = (E_{2x} + E_{4x})/(\beta H_x)$.

For $H_{x,z} = 0$ ($H_y \neq 0$), assuming $D > 0$ and $D > g_y\beta H_y$:
$E_{1y} = -(1/2)g_y\beta H_y - \{D^2 + (g_y\beta H_y)^2 + 3E^2 + D(g_y\beta H_y) + 3E(g_y\beta H_y)\}^{1/2} \rightarrow -D$ as $H_y, E \rightarrow 0$; (root #3)
$E_{2y} = (1/2)g_y\beta H_y - \{D^2 + (g_y\beta H_y)^2 + 3E^2 - D(g_y\beta H_y) - 3E(g_y\beta H_y)\}^{1/2} \rightarrow -D$ as $H_y, E \rightarrow 0$; (root #1)
$E_{3y} = -(1/2)g_y\beta H_y + \{D^2 + (g_y\beta H_y)^2 + 3E^2 + D(g_y\beta H_y) + 3E(g_y\beta H_y)\}^{1/2} \rightarrow D$ as $H_y, E \rightarrow 0$; (root #4)
$E_{4y} = (1/2)g_y\beta H_y + \{D^2 + (g_y\beta H_y)^2 + 3E^2 - D(g_y\beta H_y) - 3E(g_y\beta H_y)\}^{1/2} \rightarrow D$ as $H_y, E \rightarrow 0$; (root #2)

Thus,
$g_y = -(E_{1y} + E_{3y})/(\beta H_y)$ and $g_y = (E_{2y} + E_{4y})/(\beta H_y)$.

***S* = 2**

$S = 2$	+2	+1	0	-1	-2
+2	$2D + 2g_z\beta H_z$	$g_x\beta H_x - i\, g_y\beta H_y$	$6^{1/2} E$	0	0
+1	$g_x\beta H_x + i\, g_y\beta H_y$	$-D + g_z\beta H_z$	$(3/2)^{1/2} [g_x\beta H_x - i\, g_y\beta H_y]$	$3 E$	0
0	$6^{1/2} E$	$(3/2)^{1/2} [g_x\beta H_x + i\, g_y\beta H_y]$	$-2 D$	$(3/2)^{1/2} [g_x\beta H_x - i\, g_y\beta H_y]$	$6^{1/2} E$
-1	0	$3 E$	$(3/2)^{1/2} [g_x\beta H_x + i\, g_y\beta H_y]$	$-D - g_z\beta H_z$	$g_x\beta H_x - i\, g_y\beta H_y$
-2	0	0	$6^{1/2} E$	$g_x\beta H_x + i\, g_y\beta H_y$	$2D - 2g_z\beta H_z$

Eigenvalues ($E_{1,2,3,4,5}$, ascending value):

For $H_{x,\,y,\,z} = 0$, assuming D, $E > 0$:
$E_1 = -2(D^2 + 3E^2)^{1/2}$ (root #4)
$E_2 = -D - 3E$ (root #2)
$E_3 = -D + 3E$ (root #3)
$E_4 = 2D$ (root #1)
$E_5 = 2(D^2 + 3E^2)^{1/2}$ (root #5)
Thus,
$D = \{E_4 - (E_3 + E_2)\}/4$, and $E = (E_3 - E_2)/6$.

For $H_{x,\,y} = 0$ ($H_z \neq 0$), assuming $D > 0$ and $D > g_z\beta H_z$:
$E_{1z} = (1/3)[2D - \{(1 + 3^{1/2}i)\mathrm{A} + (1 - 3^{1/2}i)\mathrm{B}^2\}/\mathrm{B}] \rightarrow -2D$ as $H_z, E \rightarrow 0$, (root #4)
$E_{2z} = -D - \{(3E)^2 + (g_z\beta H_z)^2\}^{1/2} \rightarrow -D\ (-\ \varepsilon)$ as $H_z, E \rightarrow 0$, (root #1)
$E_{3z} = -D + \{(3E)^2 + (g_z\beta H_z)^2\}^{1/2} \rightarrow -D\ (+\ \varepsilon)$ as $H_z, E \rightarrow 0$, (root #2)
$E_{4z} = (1/3)[2D - \{(1 - 3^{1/2}i)\mathrm{A} + (1 + 3^{1/2}i)\mathrm{B}^2\}/\mathrm{B}] \rightarrow 2D$ as $H_z, E \rightarrow 0$, (root #5)
$E_{5z} = (2/3)[D + \{\mathrm{A} + \mathrm{B}^2\}/\mathrm{B}] \rightarrow 2D$ as $H_z, E \rightarrow 0$, (root #3)
where,
$\mathrm{A} = [(2D)^2 + (3E)^2 + 3(g_z\beta H_z)^2]$,
$\mathrm{B} = [-8D^3 - 27DE^2 + 18D(g_z\beta H_z)^2 + \{-\mathrm{A}^3 + [8D^3 + 27DE^2 - 18D(g_z\beta H_z)^2]^2\}^{1/2}]^{1/3}$
Thus,
$g_z = \{(E_{3z} - E_{2z})^2 - (6E)^2\}^{1/2}/(2\beta H_z)$.

For $H_{y,z} = 0$ ($H_x \neq 0$), assuming $D > 0$ and $D > g_x\beta H_x$:
$E_{1x} = (1/3)[-D + 3E - (1/2)\{(1 + 3^{1/2}i)A + (1 - 3^{1/2}i)B^2\}/B] \rightarrow -2D$ as $H_x, E \rightarrow 0$, (root #4)
$E_{2x} = (1/2)[D - 3E - \{9(D + E)^2 + (2g_x\beta H_x)^2\}^{1/2}] \rightarrow -D\ (-\ \varepsilon)$ as $H_x, E \rightarrow 0$, (root #1)
$E_{3x} = (1/3)[-D + 3E - (1/2)\{(1 - 3^{1/2}i)A + (1 + 3^{1/2}i)B^2\}/B] \rightarrow -D\ (+\ \varepsilon)$ as $H_x, E \rightarrow 0$, (root #5)
$E_{4x} = (1/2)[D - 3E + \{9(D + E)^2 + (2g_x\beta H_x)^2\}^{1/2}] \rightarrow 2D$ as $H_x, E \rightarrow 0$, (root #2)
$E_{5x} = (1/3)[-D + 3E + \{A + B^2\}/B] \rightarrow 2D$ as $H_x, E \rightarrow 0$, (root #3)
where,
$A = 13D^2 - 6DE^2 + 45E^2 + 12(g_x\beta H_x)^2$,
$B = [35D^3 - 99D^2E + 81DE^2 - 297E^3 - 72D(g_x\beta H_x)^2 + 216E(g_x\beta H_x)^2 +$
$(1/2)\{4(D^2 - 3E)^2\ [(35D^2 + 6DE^2 + 99E^2 - 72(g_x\beta H_x)^2]^2 - 4A^3\}^{1/2}]^{1/3}$.
Thus,
$g_x = \{(E_{4x} - E_{2x})^2 - 9(D + E)^2\}^{1/2}/(2\beta H_x)$.

For $H_{x,z} = 0$ ($H_y \neq 0$), assuming $D > 0$ and $D > g_y\beta H_y$:
$E_{1y} = (1/3)[-D + 3E - (1/2)\{(1 + 3^{1/2}i)A + (1 - 3^{1/2}i)B^2\}/B] \rightarrow -2D$ as $H_y, E \rightarrow 0$, (root #4)
$E_{2y} = (1/2)[D + 3E - \{9(D - E)^2 + (2g_y\beta H_y)^2\}^{1/2}] \rightarrow -D\ (-\ \varepsilon)$ as $H_y, E \rightarrow 0$, (root #1)
$E_{3y} = (1/3)[-D + 3E - (1/2)\{(1 - 3^{1/2}i)A + (1 + 3^{1/2}i)B^2\}/B] \rightarrow -D\ (+\ \varepsilon)$ as $H_y, E \rightarrow 0$, (root #5)
$E_{4y} = (1/2)[D + 3E + \{9(D - E)^2 + (2g_y\beta H_y)^2\}^{1/2}] \rightarrow 2D$ as $H_y, E \rightarrow 0$, (root #2)
$E_{5y} = (1/3)[-D + 3E + \{A + B^2\}/B] \rightarrow 2D$ as $H_y, E \rightarrow 0$, (root #3)
where,
$A = 13D^2 + 6DE^2 + 45E^2 + 12(g_y\beta H_y)^2$,
$B = [35D^3 + 99D^2E + 81DE^2 + 297E^3 - 72D(g_y\beta H_y)^2 - 216E(g_y\beta H_y)^2 +$
$(1/2)\{4(D^2 + 3E)^2\ [(35D^2 - 6DE^2 + 99E^2 - 72(g_y\beta H_y)^2]^2 - 4A^3\}^{1/2}]^{1/3}$.
Thus,
$g_y = \{(E_{4y} - E_{2y})^2 - 9(D - E)^2\}^{1/2}/(2\beta H_y)$.

***S* = 5/2**

S = 5/2	+5/2	+3/2	+1/2	-1/2	-3/2	-5/2
+5/2	$(10/3)D + g_z\beta H_z(5/2)$	$g_{xy}\beta H_x (5^{1/2}/2)$	$10^{1/2} E$	0	0	0
+3/2	$g_{xy}\beta H_x (5^{1/2}/2)$	$-(2/3)D + g_z\beta H_z(3/2)$	$g_{xy}\beta H_x(2^{1/2})$	$3\ 2^{1/2} E$	0	0
+1/2	$10^{1/2} E$	$g_{xy}\beta H_x(2^{1/2})$	$-(8/3)D + g_z\beta H_z/2$	$g_{xy}\beta H_x(3/2)$	$3\ 2^{1/2} E$	0
-1/2	0	$3\ 2^{1/2} E$	$g_{xy}\beta H_x(3/2)$	$-(8/3)D - g_z\beta H_z/2$	$g_{xy}\beta H_x(2^{1/2})$	$10^{1/2} E$
-3/2	0	0	$3\ 2^{1/2} E$	$g_{xy}\beta H_x(2^{1/2})$	$-(2/3)D - g_z\beta H_z(3/2)$	$g_{xy}\beta H_x (5^{1/2}/2)$
-5/2	0	0	0	$10^{1/2} E$	$g_{xy}\beta H_x (5^{1/2}/2)$	$(10/3)D - g_z\beta H_z(5/2)$

Use g_{xy}, H_x so only reals; rhombicity in $\boldsymbol{g}$ can be ignored for the present purposes.

Eigenvalues ($E_{1,2,3,4,5,6}$, ascending value):

For $H_{x,\,z} = 0$:
$E_{1,2} = 2\{7D^2 + 21E^2 + \mathrm{A}^2\}/\mathrm{A} \rightarrow -(8/3)D$ as $E \rightarrow 0$, (root #1,2)
$E_{3,4} = \{-7(1 - 3^{1/2}i)D^2 - 21(1 - 3^{1/2}i)E^2 - (1 + 3^{1/2}i)\mathrm{A}^2)\}/\mathrm{A} \rightarrow -(2/3)D$ as $E \rightarrow 0$, (root #3,4)
$E_{5,6} = \{-7(1 + 3^{1/2}i)D^2 - 21(1 + 3^{1/2}i)E^2 - (1 - 3^{1/2}i)\mathrm{A}^2)\}/\mathrm{A} \rightarrow (10/3)D$ as $E \rightarrow 0$, (root #5,6)
where,
$\mathrm{A} = \{10D^3 - 90DE^2 + 3\ 3^{1/2}i(9D^6 + 181D^4E^2 + 43D^2E^4 + 343E^6)^{1/2}\}^{1/3}$.

For $H_z = 0$ ($H_x \neq 0$):
E_{1x} = very complicated root $\rightarrow -(8/3)D$ as H_x, $E \rightarrow 0$, (root #5)
E_{2x} = very complicated root $\rightarrow -(8/3)D$ as H_x, $E \rightarrow 0$, (root #2)
E_{3x} = very complicated root $\rightarrow -(2/3)D$ as H_x, $E \rightarrow 0$, (root #6)
E_{4x} = very complicated root $\rightarrow -(2/3)D$ as H_x, $E \rightarrow 0$, (root #3)
E_{5x} = very complicated root $\rightarrow (10/3)D$ as H_x, $E \rightarrow 0$, (root #4)
E_{1x} = very complicated root $\rightarrow (10/3)D$ as H_x, $E \rightarrow 0$, (root #1)

We find that,
$g_{xy} = -(2/3)(E_{1x} + E_{3x} + E_{5x})/(\beta H_x)$ and $g_{xy} = (2/3)(E_{2x} + E_{4x} + E_{6x})/(\beta H_x)$.

For $H_x = 0$ ($H_z \neq 0$):
E_{1z} = very complicated root $\rightarrow$ -(8/3)D as H_z, $E \rightarrow 0$, (root #1)
E_{2z} = very complicated root $\rightarrow$ -(8/3)D as H_z, $E \rightarrow 0$, (root #2)
E_{3z} = very complicated root $\rightarrow$ -(2/3)D as H_z, $E \rightarrow 0$, (root #3)
E_{4z} = very complicated root $\rightarrow$ -(2/3)D as H_z, $E \rightarrow 0$, (root #4)
E_{5z} = very complicated root $\rightarrow$ (10/3)D as H_z, $E \rightarrow 0$, (root #5)
E_{1z} = very complicated root $\rightarrow$ (10/3)D as H_z, $E \rightarrow 0$, (root #6)

No easy combination for g_z.