John Bower

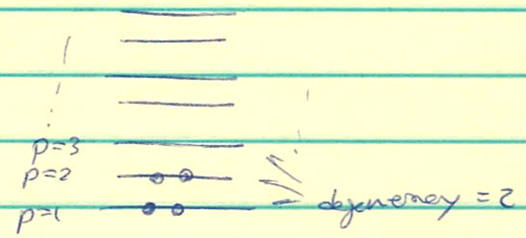
Nuclear Structure – Project 2

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \overbrace{\left(\xi \sum_{p\sigma} (p-1)\, a^\dagger_{p\sigma} a_{p\sigma}\right)}^{\hat{H}_0} + \overbrace{\left(-g \sum_{rs} a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}\right)}^{\hat{H}_1}$$

a) $\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma\, a^\dagger_{p\sigma} a_{p\sigma}$

$\hat{S}^2 = \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+)$

$\hat{S}_\pm = \sum_p a^\dagger_{p\pm} a_{p\mp}$



i) $[S_z, H] = [S_z, H_0] + [S_z, H_1]$

$[S_z, H_0] = \frac{1}{2}\xi\sigma\, [a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{p'\sigma'} a_{p'\sigma'}](p'-1)$

$= \frac{1}{2}(p'-1)\sigma\xi\, [\, a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{p'\sigma'} a_{p'\sigma'} - a^\dagger_{p'\sigma'} a_{p'\sigma'} a^\dagger_{p\sigma} a_{p\sigma}\,]$

$= \frac{1}{2}(p'-1)\sigma\xi\, (\, a^\dagger_{p\sigma}(\delta_{pp'}\delta_{\sigma\sigma'} - a^\dagger_{p'\sigma'} a_{p\sigma} a_{p'\sigma'}) a_{p'\sigma'}$

$- a^\dagger_{p'\sigma'}(\delta_{pp'}\delta_{\sigma\sigma'} - a^\dagger_{p\sigma} a_{p'\sigma'}) a_{p\sigma}\,)$

$= \frac{1}{2}(p'-1)\sigma\xi\, (\, a^\dagger_{p\sigma} a_{p'\sigma'} \delta_{pp'}\delta_{\sigma\sigma'} - a^\dagger_{p\sigma} a^\dagger_{p'\sigma'} a_{p\sigma} a_{p'\sigma'}$

$- a^\dagger_{p'\sigma'} a_{p\sigma} \delta_{pp'}\delta_{\sigma\sigma'} + \underbrace{a^\dagger_{p'\sigma'} a^\dagger_{p\sigma}}_{(-)} \underbrace{a_{p'\sigma'} a_{p\sigma}}_{(-)}$

$(+)$

$= \frac{1}{2}(p'-1)\sigma\xi\, (\, \cancel{a^\dagger_{p\sigma} a_{p\sigma}} - \cancel{a^\dagger_{p\sigma} a^\dagger_{p'\sigma'} a_{p\sigma} a_{p'\sigma'}}$

$\cancel{- a^\dagger_{p\sigma} a_{p\sigma}} + \cancel{a^\dagger_{p\sigma} a^\dagger_{p'\sigma'} a_{p\sigma} a_{p\sigma}}\,)$

$[S_z, H_0] = 0$

$[S_z, H] = 0$

$[S_z, H_1] = -\frac{1}{2} g\sigma\, [a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}]$

$= -\frac{1}{2} g\sigma\, (\, [a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{r+}] a^\dagger_{r-} a_{s-} a_{s+} + a^\dagger_{r+} [a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{r-}] a_{s-} a_{s+}$

$+ a^\dagger_{r+} a^\dagger_{r-} [a^\dagger_{p\sigma} a_{p\sigma}, a_{s-}] a_{s+} + a^\dagger_{r+} a^\dagger_{r-} a_{s-} [a^\dagger_{p\sigma} a_{p\sigma}, a_{s+}])$

$= -\frac{1}{2} g\sigma\, (\, a^\dagger_{p\sigma} \overbrace{\{a_{p\sigma}, a^\dagger_{r+}\}}^{\delta_{pr}\delta_{\sigma+}} a^\dagger_{r-} a_{s-} a_{s+} - \cancel{\{a^\dagger_{p\sigma}, a^\dagger_{r+}\} a_{p\sigma} a^\dagger_{r-} a_{s-} a_{s+}}$

$+ a^\dagger_{r+} a^\dagger_{p\sigma} \overbrace{\{a_{p\sigma}, a^\dagger_{r-}\}}^{\delta_{pr}\delta_{\sigma-}} a_{s-} a_{s+} - \cancel{a^\dagger_{r+} \{a^\dagger_{p\sigma}, a^\dagger_{r-}\} a_{p\sigma} a_{s-} a_{s+}}$

$+ \cancel{a^\dagger_{r+} a^\dagger_{r-} a^\dagger_{p\sigma} \{a_{p\sigma}, a_{s-}\} a_{s+}} - a^\dagger_{r+} a^\dagger_{r-} \overbrace{\{a^\dagger_{p\sigma}, a_{s-}\}}^{\delta_{ps}\delta_{\sigma-}} a_{p\sigma} a_{s+}$

$+ \cancel{a^\dagger_{r+} a^\dagger_{r-} a_{s-} a^\dagger_{p\sigma} \{a_{p\sigma}, a_{s+}\}} - a^\dagger_{r+} a^\dagger_{r-} a_{s-} \overbrace{\{a^\dagger_{p\sigma}, a_{s+}\}}^{\delta_{ps}\delta_{\sigma+}} a_{p\sigma})$

$= -\frac{1}{2} g\sigma\, (\, \cancel{a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}} + \cancel{a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}} - \cancel{a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}} - \cancel{a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}}$

$[S_z, H_1] = 0$

$[S_\pm, H] = [S_\pm, H_0 + H_1]$

$$[S_\pm, H_0] = \xi(p-1)\,[a^\dagger_{p'\pm} a_{p'\mp}, a^\dagger_{p\sigma} a_{p\sigma}]$$
$$= \xi(p-1)\left([a^\dagger_{p'\pm} a_{p'\mp}, a^\dagger_{p\sigma}] a_{p\sigma} + a^\dagger_{p\sigma} [a^\dagger_{p'\pm} a_{p'\mp}, a_{p\sigma}] \right)$$
$$= \xi(p-1)\Big(a^\dagger_{p'\pm}\{a_{p'\mp}, a^\dagger_{p\sigma}\} a_{p\sigma} - \cancel{\{a^\dagger_{p'\pm}, a^\dagger_{p\sigma}\} a_{p'\mp} a_{p\sigma}}$$
$$+ \cancel{a^\dagger_{p\sigma} a^\dagger_{p'\pm}\{a_{p'\mp}, a_{p\sigma}\}} - a^\dagger_{p\sigma}\{a^\dagger_{p'\pm}, a_{p\sigma}\} a_{p'\mp} \Big)$$
$$= \xi(p-1)\left(a^\dagger_{p'\pm} a_{p\sigma} \delta_{pp'} \delta_{\sigma\mp} - a^\dagger_{p\sigma} a_{p'\mp} \delta_{pp'} \delta_{\sigma\pm} \right)$$
$$= \xi(p-1)\left(\cancel{a^\dagger_{p\pm} a_{p\mp}} - \cancel{a^\dagger_{p\pm} a_{p\mp}} \right) = 0$$

$[S_\pm, H_0] = 0$

$$[S_\pm, H_1] = -g\,[a^\dagger_{p\pm} a_{p\mp}, a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s+}]$$
$$= -g\Big([a^\dagger_{p\pm} a_{p\mp}, a^\dagger_{r+}] a^\dagger_{r-} a_{s-} a_{s+} + a^\dagger_{r+} [a^\dagger_{p\pm} a_{p\mp}, a^\dagger_{r-}] a_{s-} a_{s+}$$
$$+ a^\dagger_{r+} a^\dagger_{r-} [a^\dagger_{p\pm} a_{p\mp}, a_{s-}] a_{s+} + a^\dagger_{r+} a^\dagger_{r-} a_{s-} [a^\dagger_{p\pm} a_{p\mp}, a_{s+}] \Big)$$
$$= -g\Big(\left(a^\dagger_{p\pm}\{a_{p\mp}, a^\dagger_{r+}\} - \cancel{\{a^\dagger_{p\pm}, a^\dagger_{r+}\} a_{p\mp}}\right) a^\dagger_{r-} a_{s-} a_{s+}$$
$$+ a^\dagger_{r+}\left(a^\dagger_{p\pm}\{a_{p\mp}, a^\dagger_{r-}\} - \cancel{\{a^\dagger_{p\pm}, a^\dagger_{r-}\} a_{p\mp}} \right) a_{s-} a_{s+}$$
$$+ a^\dagger_{r+} a^\dagger_{r-}\left(\cancel{a^\dagger_{p\pm}\{a_{p\mp}, a_{s-}\}} - \{a^\dagger_{p\pm}, a_{s-}\} a_{p\mp} \right) a_{s+}$$
$$+ a^\dagger_{r+} a^\dagger_{r-} a_{s-}\left(\cancel{a^\dagger_{p\pm}\{a_{p\mp}, a_{s+}\}} - \{a^\dagger_{p\pm}, a_{s+}\} a_{p\mp} \right) \Big)$$
$$= -g\Big(a^\dagger_{p\pm} a^\dagger_{r-} a_{s-} a_{s+} \delta_{pr} \delta_{\mp +} + a^\dagger_{r+} a^\dagger_{p\pm} a_{s-} a_{s+} \delta_{pr} \delta_{\mp -}$$
$$- (a^\dagger_{r+} a^\dagger_{r-} a_{p\mp} a_{s+} \delta_{ps} \delta_{\pm -}) - (a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{p\mp} \delta_{ps} \delta_{\pm +}) \Big)$$
$$= -g\Big[\delta_+ \left(\sum_s a^\dagger_{r+} a^\dagger_{r+} a_{s-} a_{s+} - \sum_r a^\dagger_{r+} a^\dagger_{r-} a_{s-} a_{s-} \right)$$
$$+ \delta_- \left(\sum_s a^\dagger_{r-} a^\dagger_{r-} a_{s-} a_{s+} - a^\dagger_{r+} a^\dagger_{r-} a_{s+} a_{s+} \right) \Big]$$

$[S_\pm, H_1] = 0$

Note in this final step we have made explicit which sums remain, though it is unnecessary. The δ_+ and δ_- refer to S_+ and S_- respectively. Each of these terms individually is zero since each either attempts to creation or destroy the same particle twice in a row, i.e. $a^\dagger_{r+} a^\dagger_{r+}$, $a_{s-} a_{s-}$, $a^\dagger_{r-} a^\dagger_{r-}$, and $a_{s+} a_{s+}$, respective to their order ①②.

Thus, $[S_\pm, H_1] = 0$.

Since $\hat{S}^2 = \hat{S}_z^2 + (S_+ S_- + S_- S_+)$, we may also then say

$[\hat{S}^2, H] = 0$.

$\sum_p [P_p^+ P_p^-, H]$.

We wish to show the above. Further, it can be reasoned conceptually but we will show that $[P_p^+ P_q^-, H]=0$ only for $p=q$.

$$[P_p^+ P_q^-, H_0] = [a^+_{p+} a^+_{p-} a_{q-} a_{q+}, \sum (r-1) a^+_{r\sigma} a_{r\sigma}] \quad \text{sum over } r,\sigma$$

$$= \sum (r-1) \Big([a^+_{p+}, a^+_{r\sigma} a_{r\sigma}] a^+_{p-} a_{q-} a_{q+} + a^+_{p+}[a^+_{p-}, a^+_{r\sigma}a_{r\sigma}] a_{q-}a_{q+}$$
$$+ a^+_{p+}a^+_{p-}[a_{q-}, a^+_{r\sigma}a_{r\sigma}]a_{q+} + a^+_{p+}a^+_{p-}a_{q-}[a_{q+}, a^+_{r\sigma}a_{r\sigma}] \Big)$$

$$= \sum(r-1)\Big(\cancel{\{a^+_{p+}, a^+_{r\sigma}\} a_{r\sigma} a^+_{p-} a_{q-} a_{q+}} - a^+_{r\sigma}\{a^+_{p+}, a_{r\sigma}\} a^+_{p-}a_{q-}a_{q+}$$
$$+ \cancel{a^+_{p+}\{a^+_{p-}, a^+_{r\sigma}\} a_{r\sigma} a_{q-} a_{q+}} - a^+_{p+}a^+_{r\sigma}\{a^+_{p-}, a_{r\sigma}\} a_{q-}a_{q+}$$
$$+ a^+_{p+}a^+_{p-}\{a_{q-}, a^+_{r\sigma}\} a_{r\sigma}a_{q+} - \cancel{a^+_{p+}a^+_{p-}a^+_{r\sigma}\{a_{q-}, a_{r\sigma}\}a_{q+}}$$
$$+ a^+_{p+}a^+_{p-}a_{q-}\{a_{q+}, a^+_{r\sigma}\}a_{r\sigma} - \cancel{a^+_{p+}a^+_{p-}a_{q-}a^+_{r\sigma}\{a_{q+}, a_{r\sigma}\}}\Big)$$

$$= \sum(r-1)\Big(-a^+_{r\sigma}a^+_{p-}a_{q-}a_{q+}\delta_{pr}\delta_{+\sigma} - a^+_{p+}a^+_{r\sigma}a_{q-}a_{q+}\delta_{rp}\delta_{\sigma-}$$
$$+ a^+_{p+}a^+_{p-}a_{r\sigma}a_{q+}\delta_{rq}\delta_{\sigma-} + a^+_{p+}a^+_{p-}a_{q-}a_{r\sigma}\delta_{rq}\delta_{\sigma+}\Big)$$

sum is lost to δ_{pr}/δ_{qr}

$$= \sum\Big[-(p-1)a^+_{p+}a^+_{p-}a_{q-}a_{q+} - (p-1)a^+_{p+}a^+_{p-}a_{q-}a_{q+}$$
$$+(q-1)a^+_{p+}a^+_{p-}a_{q-}a_{q+} + (q-1)a^+_{p+}a^+_{p-}a_{q-}a_{q+}\Big]$$

$$= 2\sum a^+_{p+}a^+_{p-}a_{q-}a_{q+}(q-p) \longrightarrow 0 \text{ if } p=q.$$

This makes good sense because an exchange of a pair from $p\to q$ would change the energy.

Now we show $[\sum_p P_p^+P_p^-, H_1]=0$.

$$-g[\sum_p P_p^+P_p^-, \sum_{rs} P_r^+P_s^-] = -g\sum_{prs}[P_p^+P_p^-, P_r^+P_s^-] \longrightarrow \text{sum to be omitted for now.}$$

$$= -g\sum_{rp}\big([P_p^+P_p^-, P_r^+]P_s^- + P_r^+[P_p^+P_p^-, P_s^-]\big)$$

$$= -g\sum_{rsp}\big(P_p^+[P_p^-, P_r^+]P_s^- + [P_p^+, P_r^+]P_p^-P_s^- + P_r^+P_p^+[P_p^-, P_s^-] + P_r^+[P_p^+, P_s^-]P_p^-\big)$$

Now $[P_m^\pm, P_r^\pm]=0$ since $a^\pm_{m+}a^\pm_{m-}a^\pm_{n-}a^\pm_{n+} = a^\pm_{n-}a^\pm_{n+}a^\pm_{m+}a^\pm_{m-}$ due to the number of interchanges being even.

Next $[P_m^+, P_n^-] = [a^+_{m+}a^+_{m-}, a_{n-}a_{n+}] = [a^+_{m+}a^+_{m-}, a_{n-}]a_{n+} + a_{n-}[a^+_{m+}a^+_{m-}, a_{n+}]$

$$= a^+_{m+}\{a^+_{m-}, a_{n-}\}a_{n+} - \cancel{\{a^+_{m+}, a_{n-}\}a^+_{m-}a_{n+}} + \cancel{a_{n-}a^+_{m+}\{a^+_{m-}, a_{n+}\}}$$
$$- a_{n-}\{a^+_{m+}, a_{n+}\}a^+_{m-}$$

$$[P_m^+, P_n^-] = a_{m+}^+ a_{n+} \delta_{mn} - a_{n-} a_{m-}^+ \delta_{mn} = (a_{m+}^+ a_{m+} - a_{m-} a_{m-}^+)\delta_{mn}$$

and similarly

$$[P_m^\pm, P_n^\mp] = \delta_{mn} (\pm)(a_{m+}^+ a_{m+} - a_{m-} a_{m-}^+)$$

Thus

$$-g \sum_{rps} [P_p^+ P_p^-, P_r^+ P_s^-] = -g \sum_{prs} \Big(P_p^+ [P_p^-, P_r^+] P_s^- + \cancel{[P_p^+, P_r^+] P_p P_s^-} + \cancel{P_r^+ P_p^+ [P_p, P_s^-]}$$
$$+ P_r^+ [P_p^+, P_s^-] P_p^- \Big)$$

$$= -g \sum_{rps} \left(-P_p^+ [P_r^+, P_p^-] P_s^- + P_r^+ [P_p^+, P_s^-] P_p^- \right)$$

$$= -g \sum_{rps} \left(P_r^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_p^- \delta_{ps} - P_p^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_s^- \delta_{pr} \right)$$

$$= -g \left(\sum_p \left(\sum_r P_r^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_p^- - \sum_s P_p^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_s^- \right)\right)$$

convert label $r \to s$

$$= -g \sum_{ps} \left(P_s^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_p^- - P_p^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_s^- \right)$$

switch labels in second sum.

$$= -g \sum_{ps} \left(P_s^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+) P_p^- - P_s^+ (a_{s+}^+ a_{s+} - a_{s-} a_{s-}^+) P_p^- \right)$$
$$= -g \sum_{ps} \left(P_s^+ (a_{p+}^+ a_{p+} - a_{p-} a_{p-}^+ - a_{s+}^+ a_{s+} + a_{s-} a_{s-}^+) P_p^- \right)$$
$$= -g \sum_{ps} \left(P_s^+ (a_{p+}^+ a_{p+} + a_{p-}^+ a_{p-} - a_{s+}^+ a_{s+} - a_{s-}^+ a_{s-}) P_p^- \right)$$

Note this breaks into four cases (technically more, but will come to that). Namely the following:

$1 \to$ yes (occ.)

$0 \to$ no (empty)

p	s	
0	0	1
1	0	2
0	1	3
1	1	4

Cases ~~2~~ 1 and 3 clearly go to zero as we attempt to destroy a pair which doesn't exist. Case two is zero since all operates after P_p^- destroy a particle in either p or s, both empty. Case 4 is zero since applying P_p^-

results in $p=0, r=1$. Thus only the last two terms may act, leaving only $P_r^+(-|p=0, r=1\rangle)=0$ as we create a pair where one exists. The only case left (the "fifth") is $p=1$, r having only an unpaired particle. This is similar to case four except now only term 3 or 4 survive and we finally attempt to create either an a_{r+}^+ or a_{r-}^+ again.

Thus we may say

$$\sum_p [P_p^+ P_p^-, H_1] = 0.$$

So $\sum_p [P_p^+ P_p^-, H] = 0$, as desired.

b)

$$H = \begin{array}{c|cc} & |1\rangle & |2\rangle \\ \hline \langle 1| & -g & -g \\ \langle 2| & -g & 2\xi - g \end{array} \xrightarrow{\xi = 1} \begin{pmatrix} -g & -g \\ -g & 2-g \end{pmatrix}$$

Then $E_\pm = 1 - g \pm \sqrt{1+g^2}$

Analytic

g	E_+	E_-
1	$\sqrt{2}$	$-\sqrt{2}$
1/2	$1/2 + \frac{\sqrt{5}}{2}$	$1/2 - \frac{\sqrt{5}}{2}$
0	2	0
$-\frac{1}{2}$	$\frac{3+\sqrt{5}}{2}$	$\frac{3-\sqrt{5}}{2}$
-1	$2+\sqrt{2}$	$2-\sqrt{2}$

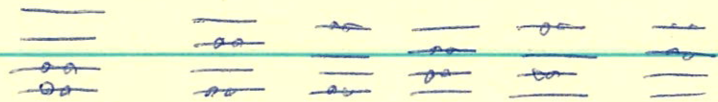
$E_0 = gs$

decimal

g	E_+	E_-
1	1.41	-1.41
1/2	1.62	-0.62
0	2	0
$-\frac{1}{2}$	2.62	0.38
-1	3.41	0.59

$E_0 = gs$

We see that for positive g we have an attractive interaction and so the system is bound. For $g < 0$, the system is unbound; since $E_- = E_0 \geq 0$

c) 

$|1\rangle$ $|2\rangle$ $|3\rangle$ $|4\rangle$ $|5\rangle$ $|6\rangle$

$\langle 1|$	$2-2g$	$-g$	$-g$	$-g$	$-g$	0
$\langle 2|$	$-g$	$4-2g$	$-g$	$-g$	0	$-g$
$\langle 3|$	$-g$	$-g$	$6-2g$	0	$-g$	$-g$
$\langle 4|$	$-g$	$-g$	0	$6-2g$	$-g$	$-g$
$\langle 5|$	$-g$	0	$-g$	$-g$	$8-2g$	$-g$
$\langle 6|$	0	$-g$	$-g$	$-g$	$-g$	$10-2g$

g	E_0 (GS.)	E_1	E_2	E_3	E_4	E_5
1	-1.49	2	4	4	6.79	8.70
1/2	0.68	2.94	5	5	7.21	9.22
0	2	4	6	6	8	10
-1/2	2.78	4.79	7	7	9.06	11.36
-1	3.30	5.21	8	8	10	13.49

Here we similar to b) that for ~~some~~ $g=1$, we have a bound system. However in contrast we see that the interaction must be of sufficient strength in addition to being negative for a bound system, $E_0 < 0$.

d)/e) The code is found on github.
→ johnbower2012/PHY981_work/project2

The code reproduces exactly the energies for b) and c). Given an input of ~~num~~
- $p \rightarrow$ number of levels
- $\Omega \rightarrow$ degeneracy of each level
- $m \rightarrow$ particles
- $g \rightarrow$ interaction energy.

for pairing case → outfile → outfile for hamiltonian
→ infile → read same as outfile, or input a custom matrix to diagonalize.

Note that for pairing we ~~need~~ reduce $\Omega \rightarrow \Omega/2$ and $m \rightarrow m/2$ to treat them as single particles.

Thus 2 levels, 2 deg, 2 particles → 2 1 1.
4 ″, 2 ″, 4 ″ → 4 1 2.
6 ″, 2 ″, 6 ″ → 6 1 3
etc.

To calculate $\boxed{E_0 = -\frac{g}{4} n(\Omega - n + 2)}$ change

$p=2, \Omega=2, m=2$ $\xrightarrow{\text{pairs}}$ $p = 2$, deg $= 1$, $m=1$ particles → $p=1, \Omega=2, m=1$
$p=4, \Omega=2, m=4$ $= 4$, deg $= 1$, $m=2$ → $p=1, \Omega=4, m=2$
etc.

With this we reproduce E_0 as follows.

g	$p=2$	$p=4$	$p=6$	$p=8$
1	-2	-6	-12	-20
1/2	-1	-3	-6	-10
0	0	0	0	0
-1/2	0	0	0	0
-1	0	0	0	0