5.3 Diagram rules with examples.

a) Definitions

We will use what are labelled as Hugenholtz vertices, defined by a two-particle operator

$$\hat{V} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{\gamma}$$

where $v_{\alpha\beta\gamma\delta} = \langle 0 | a_{\beta} a_{\alpha} V a^{\dagger}_{\gamma} a^{\dagger}_{\delta} | 0 \rangle$

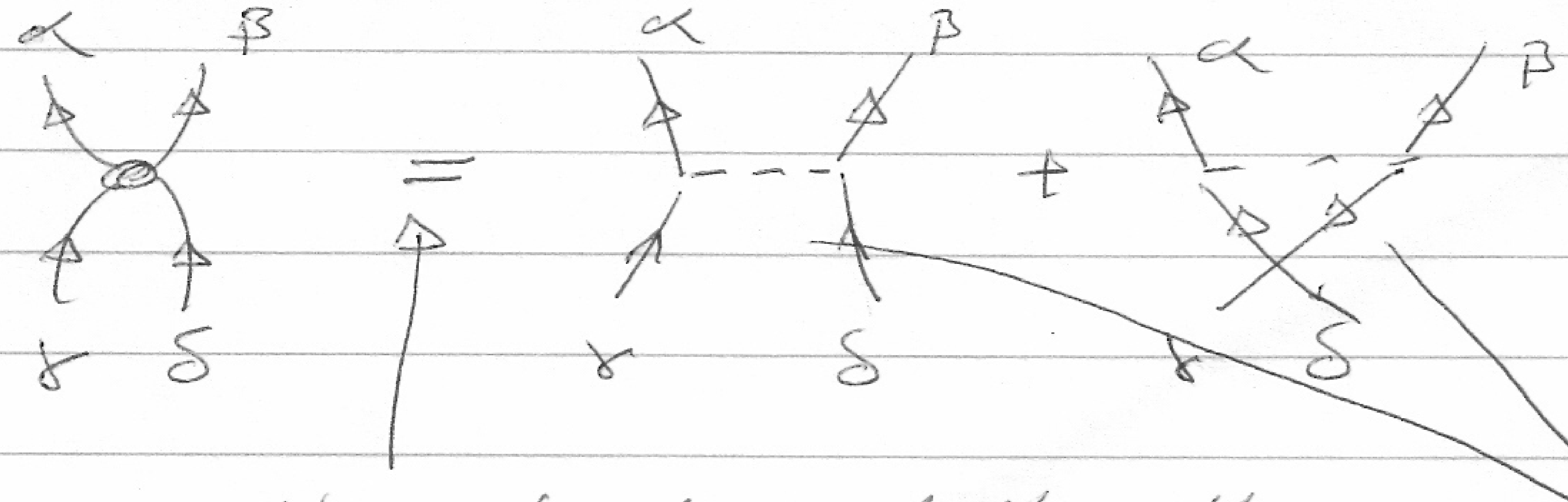
that is, a c-number.

The element $v_{\alpha\beta\gamma\delta}$ has the property that

$$v_{\alpha\beta\gamma\delta} = -v_{\alpha\beta\delta\gamma} = -v_{\beta\alpha\gamma\delta}$$

$$= v_{\beta\alpha\delta\gamma}$$

It contains both the direct and the exchange term. It is normally depicted as



These are called Goldstone diag.

It includes both the direct term and the exchange term

The notation $v_{\alpha\beta\gamma\delta}$ is rather compact.
It can therefore be useful to rewrite it as

$$v_{\alpha\beta\gamma\delta} = \langle\alpha\beta|v|\gamma\delta\rangle - \langle\alpha\beta|v|\delta\gamma\rangle$$

$$= \langle\alpha\beta|v|\gamma\delta\rangle_{AS}$$

one sees that interchanging the labels $\gamma \leftrightarrow \delta$ gives

$$v_{\alpha\beta\delta\gamma} = \langle\alpha\beta|v|\delta\gamma\rangle - \langle\alpha\beta|v|\gamma\delta\rangle$$

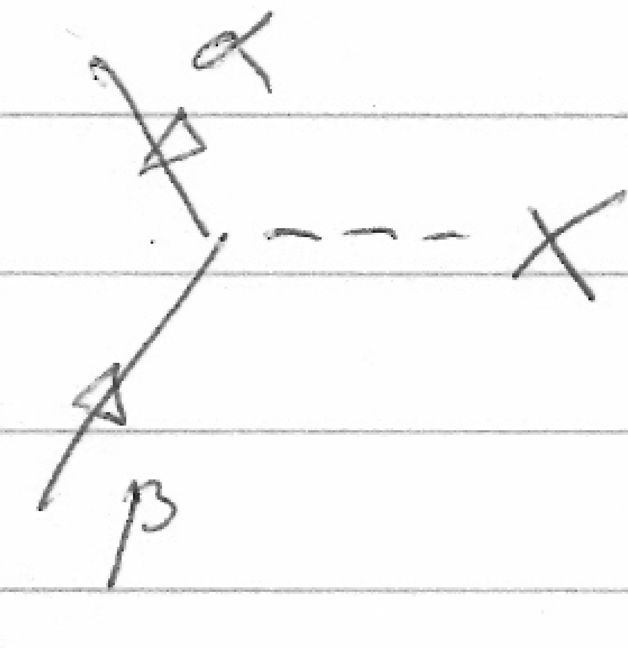
which is nothing but $-v_{\alpha\beta\gamma\delta}$

The Hamiltonian has also a onebody part which can be included in H_I, that is $\hat{H}_I = \hat{V} + \hat{u}$

$$\hat{u} = \sum_{\alpha\beta} \langle\alpha|u|\beta\rangle a^{\dagger}_{\alpha} a_{\beta}$$

it is not necessarily diagonal in the single-particle basis.

it is drawn as



particle lines are drawn as 

hole 

The expectation value of the energy is given by $E - E_0 = \Delta E = \sum_{n=0}^{\infty} (\Delta E)^{(n+1)}$

with

$$
(\Delta E)^{(n+1)} = \lim_{\varepsilon \to 0^+} \left(\frac{i}{\hbar}\right)^n \langle \Phi_0 | H_I(t=0)
\times \int_{-\infty}^{0} e^{n\varepsilon t_1} e^{i(H_0 - E_0)t_1/\hbar} dt_1 \, H_I
\times \int_{-\infty}^{0} e^{(n-1)\varepsilon t_2} e^{i(H_0 - E_0)t_2/\hbar} dt_2 \, H_I
\cdots \times \int_{-\infty}^{0} e^{\varepsilon t_n} e^{i(H_0 - E_0)t_n/\hbar} dt_n \, H_I | \Phi_0 \rangle
$$

where only linked diagrams are included.

To first order we have $(n=0)$

$$\Delta E_0^{(1)} \langle \Phi_0 | H_I(t=0) | \Phi_0 \rangle$$

$$= \langle \Phi_0 | \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

$$\times e^{-i(\varepsilon_\delta + \varepsilon_\gamma - \varepsilon_\alpha - \varepsilon_\beta + i\varepsilon)t/\hbar} |\Phi_0\rangle$$

$\uparrow$ $t=0$

The states are all hole states, we can therefore just limit ourselves to hole-hole contractions

$$a_\alpha^+ a_\beta^+ a_\delta a_\gamma$$

(contractions: a_β^+ with a_δ, a_α^+ with a_γ)

every such contraction gives a factor (-1), That is, we get a general factor $(-)^{n_h}$, n_h = # holes

The other contraction is

$$a_\alpha^+ a_\beta^+ a_\delta a_\gamma = - a_\beta^+ a_\alpha^+ a_\delta a_\gamma$$

(contractions: a_α^+ with a_δ, a_β^+ with a_γ; on the right: a_α^+ with a_δ, a_β^+ with a_γ)

$\uparrow$ group them together

In the first contraction the two hole pair are grouped together. That is we have two pairs of holes,

We shall see below that this regrouping gives rise to an additional factor $(-1)^{n_e}$

n_e = number of loops in a diagram

The first contraction gives

$$\delta_{\beta\delta}\,\delta_{\alpha\gamma} \rightarrow v_{\alpha\beta\alpha\beta}$$

The second contraction gives

$$-\delta_{\beta\gamma}\,\delta_{\alpha\delta} \rightarrow -v_{\alpha\beta\beta\alpha} = v_{\alpha\beta\alpha\beta}$$

we get therefore the following contribution to the energy

$$\frac{1}{2}\sum_{\alpha\beta\leq F} v_{\alpha\beta\alpha\beta} =$$

$$\frac{1}{2}\sum_{\alpha\beta\leq F}\left\{\langle\alpha\beta|v|\alpha\beta\rangle - \langle\alpha\beta|v|\alpha\beta\rangle\right\}$$

a well-known result.

Diagrammatically we can draw this in the Hugenholtz notation as

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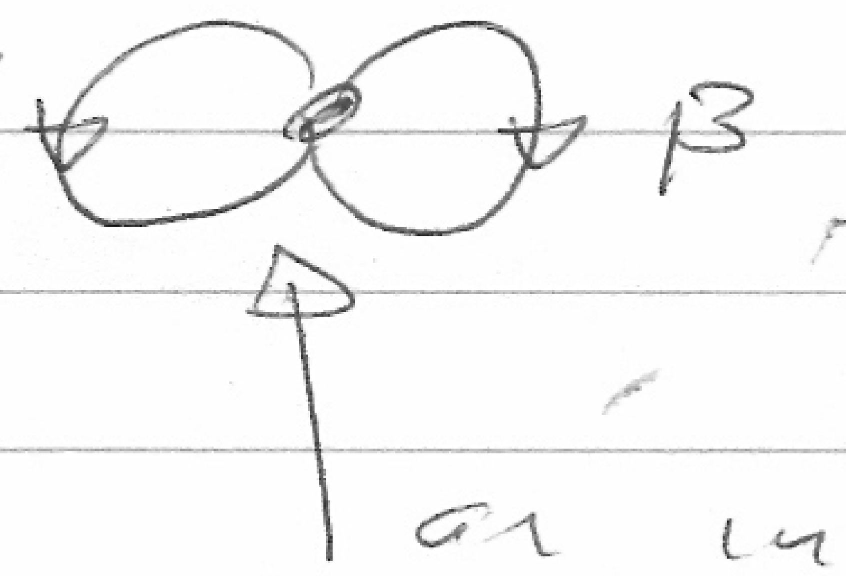
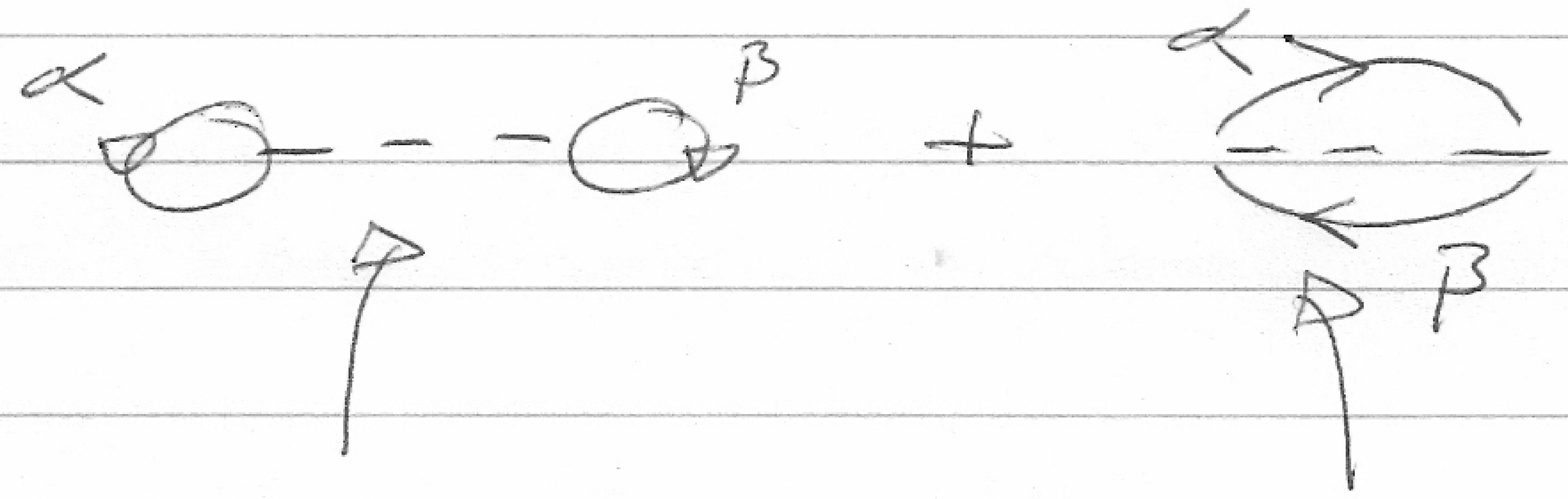
$\frac{1}{2}\sum_{\alpha\beta\gamma\delta}$  ,

as in the Goldstone formalism as



$\langle\alpha\beta|v|\alpha\beta\rangle \qquad - \langle\alpha\beta|v|\beta\alpha\rangle$

In each diagram we have

2 hole lines $n_h = 2 \Rightarrow (-)^2 = +\underline{1}$

In the first diagram we grouped the pairs of holes as $a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$

each pair gives rise to a loop.
we have therefore $n_\ell = +2 \Rightarrow$
in total our factor becomes

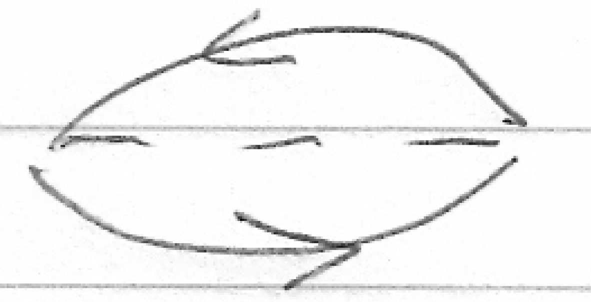
$(-)^{n_\ell + n_h} = (-)^4 = +\underline{1}$

In the second diagram we

have regrouped the pairs from

$$a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = - a_\beta^\dagger a_\alpha^\dagger a_\delta a_\gamma$$

this regrouping closes fermion lines
however the diagram has now
only one loop, that is



is counted as
one loop only.

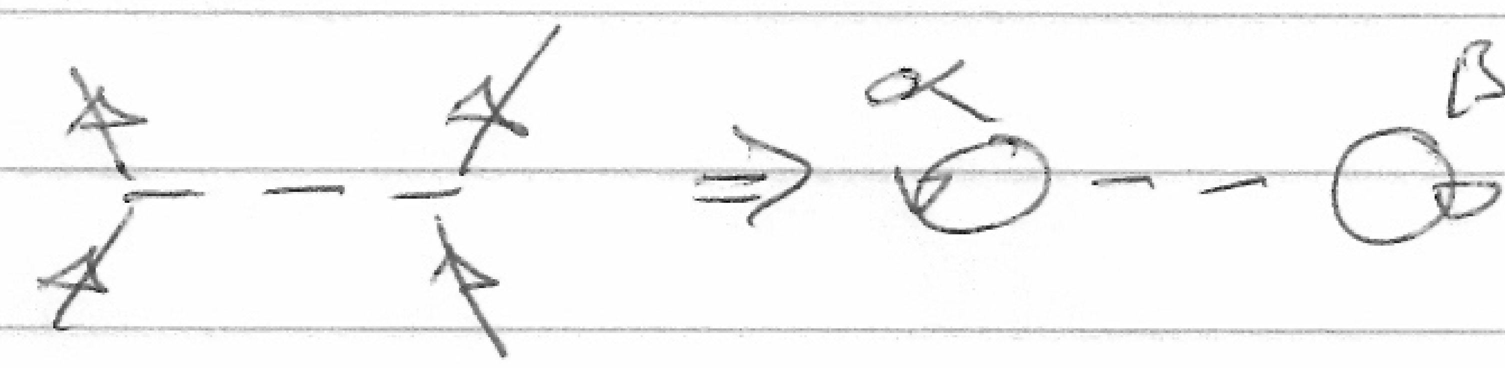
NOTE : you will get the same
result if you use Goldstone
diagrams. Then we have

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

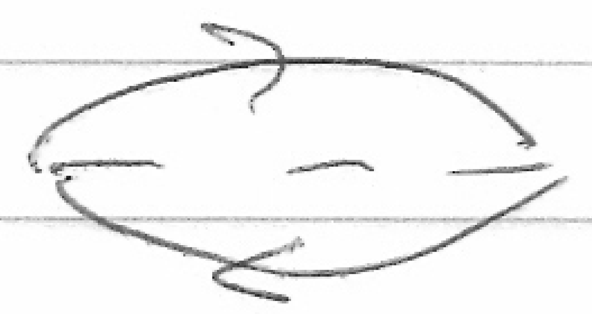
The contractions yield the same
results as previously, but now

we have a matrix element

$\langle \alpha\beta | v | \alpha\beta \rangle =$



and $\langle \alpha\beta | v | \beta\alpha \rangle =$



The final result is obviously the same, namely

$$(\Delta E) = \frac{1}{2}\sum_{\alpha\beta}\left\{\langle\alpha\beta|V|\alpha\beta\rangle - \langle\alpha\beta|V|\beta\alpha\rangle\right\}$$

the factor comes from the definition of the operator $\hat{V}$.

In summary: you can choose between what are called Goldstone diagrams with

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

or so-called Hugenholtz diagrams with

$$\hat{V} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

$$v_{\alpha\beta\gamma\delta} = \langle\alpha\beta|V|\gamma\delta\rangle - \langle\alpha\beta|V|\delta\gamma\rangle$$

The latter is more convenient from a computational perspective since we include both the direct term and the exchange term.

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To second order we have the following term $(n=1)$

$$(\Delta E)^{(2)} = \lim_{\varepsilon \to 0^+} \langle \Phi_0 | H_I(t=0) \left(\frac{-i}{\hbar}\right) \int_{-\infty}^{0} e^{\varepsilon t_1} H_I(t_1)$$

$$\times | \Phi_0 \rangle$$

$$H_I(t_1) = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma v_{\alpha\beta\gamma\delta}$$
$$\times e^{-i(\varepsilon_\delta + \varepsilon_\gamma - \varepsilon_\alpha - \varepsilon_\beta) t_1/\hbar}$$

Let us look at the contractions

$$(a_\sigma^\dagger a_\lambda^\dagger a_\nu a_\mu)_{t=0} \, (a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma)_{t=t_1}$$

|| We cannot have unlinked diagrams. This means that at least one of the operators at $t=0$ and one at $t=t_1$ need to be contracted.

We consider just the case that ~~the~~ operators from $t=0$ are contracted with all operators from $t=t_1$. That is we have now

$$a^\dagger_\sigma a^\dagger_\gamma a_\nu a_\mu \; a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

These must be particle states

these must be hole states

In total we have 4 possibilities:

(i) $\delta_{\mu\alpha}\delta_{\nu\beta}\delta_{\gamma\delta}\delta_{\sigma\gamma}$ → 2 hole lines and two pairs of holes (two loops)

(ii) $-\delta_{\mu\beta}\delta_{\alpha\nu}$ — " — → 2 hole lines but only one loop.

(iii) $+\delta_{\mu\beta}\delta_{\alpha\nu}\delta_{\gamma\gamma}\delta_{\sigma\delta}$ 2 hole lines and two loops

(iv) $-\delta_{\mu\alpha}\delta_{\nu\beta}\delta_{\gamma\gamma}\delta_{\sigma\delta}$ 2 hole lines and one loop.

The matrix elements are

(i) $v_{\gamma\delta\alpha\beta}\, v_{\alpha\beta\gamma\delta}$ $\quad \gamma\delta \le F$, $\alpha\beta > F$

(ii) $-v_{\gamma\delta\beta\alpha}\, v_{\beta\alpha\gamma\delta}$ — " —

$= +v_{\gamma\delta\alpha\beta}\, v_{\alpha\beta\gamma\delta}$

(iii) $v_{\delta\gamma\beta\alpha} v_{\alpha\beta\gamma\delta} = v_{\gamma\delta\alpha\beta} v_{\alpha\beta\gamma\delta}$

that is it is identical to (i)

(iv) $-v_{\gamma\delta\alpha\beta} v_{\alpha\beta\delta\gamma} = +v_{\gamma\delta\alpha\beta} v_{\alpha\beta\delta\gamma}$

We get four contributions which read $v_{\gamma\delta\alpha\beta} v_{\alpha\beta\delta\gamma}$ =>

$$(\Delta E)^{(2)} = 4 \frac{1}{16} \sum_{\substack{\alpha\beta > F \\ \gamma\delta \leq F}} v_{\gamma\delta\alpha\beta} v_{\alpha\beta\delta\gamma}$$

The time integration gives a factor

$$\frac{1}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_\alpha - \varepsilon_\beta}$$

In total we have

$$\frac{1}{4} \sum_{\substack{\alpha\beta > F \\ \gamma\delta \leq F}} \frac{|v_{\gamma\delta\alpha\beta}|^2}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_\alpha - \varepsilon_\beta}$$

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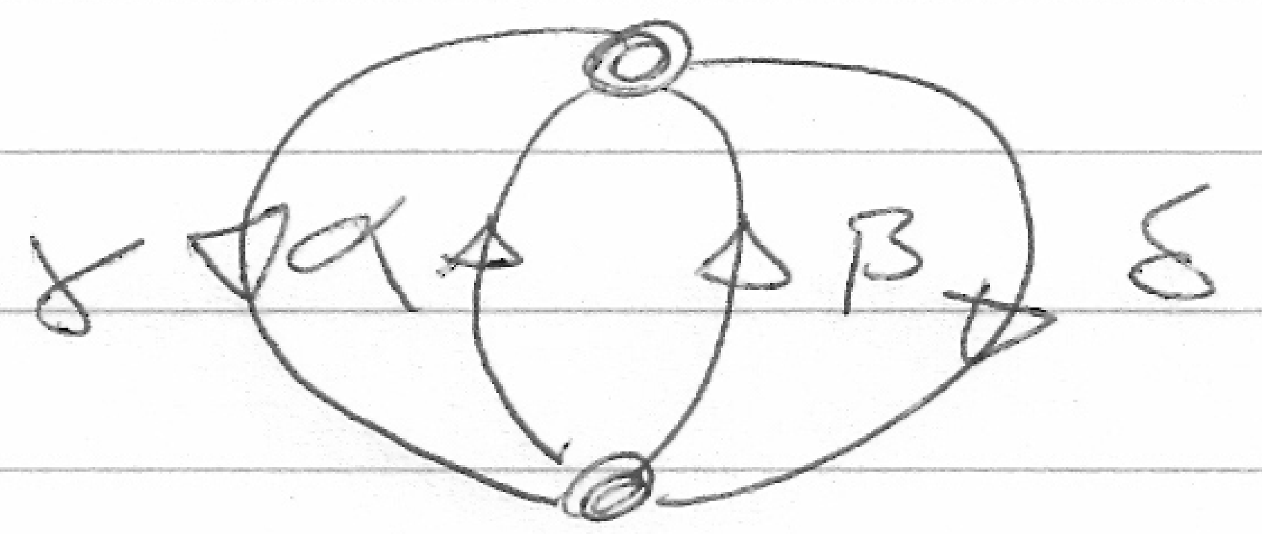
we can write the expression for this diagram as



if we write it out as Goldstone diagrams we need to remember that we have

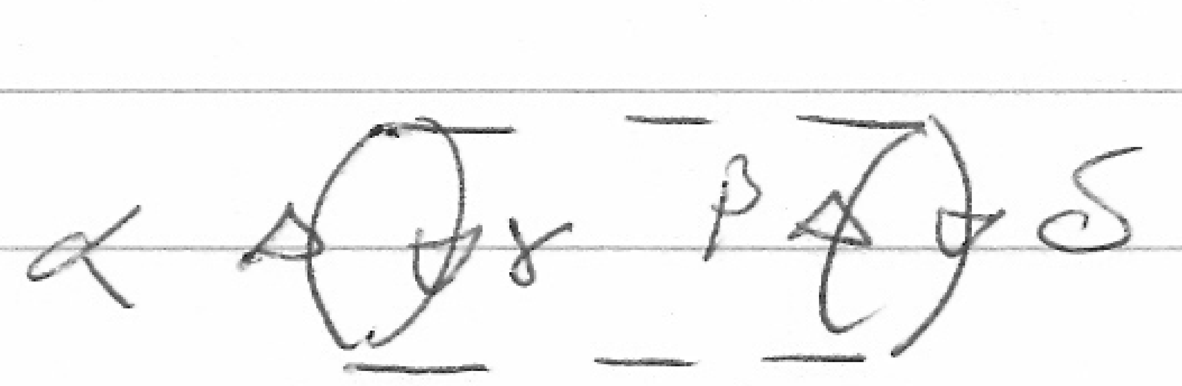
$$|v_{\gamma\delta\alpha\beta}|^2 =$$

$$(\langle\gamma\delta|v|\alpha\beta\rangle - \langle\gamma\delta|v|\beta\alpha\rangle)$$

$$\times (\langle\alpha\beta|v|\gamma\delta\rangle - \langle\alpha\beta|v|\delta\gamma\rangle)$$

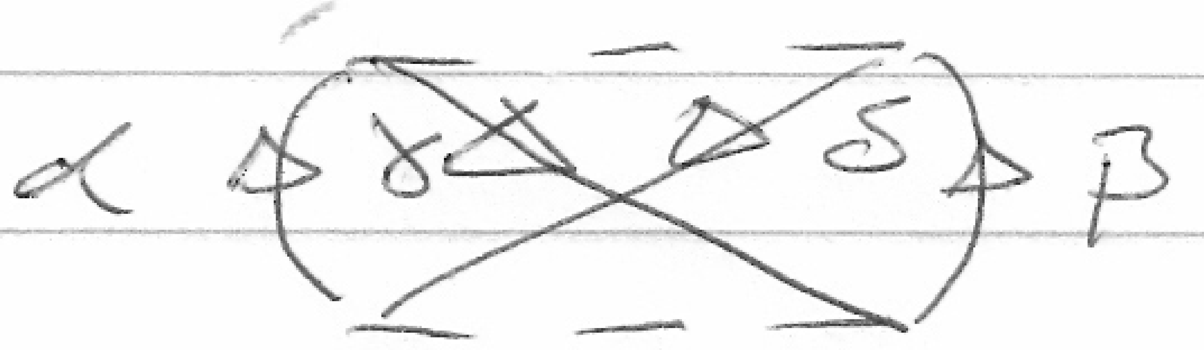
we get four diagrams (the four contractions)

(i) $\langle\gamma\delta|v|\alpha\beta\rangle\langle\alpha\beta|v|\gamma\delta\rangle$



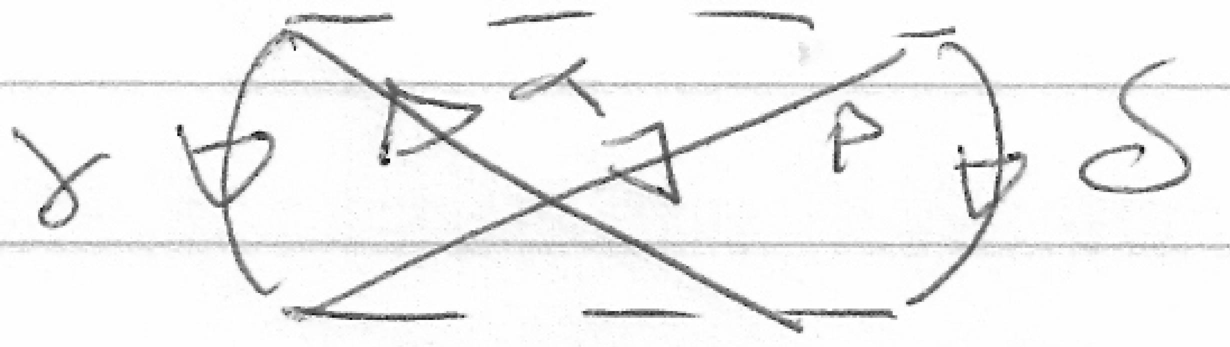
2 holes
2 loops

(ii) $-\langle \gamma\delta | v | \alpha\beta \rangle \langle \alpha\beta | v | \delta\gamma \rangle$



2 holes
one loop
$(-)^{2+1} = -1$

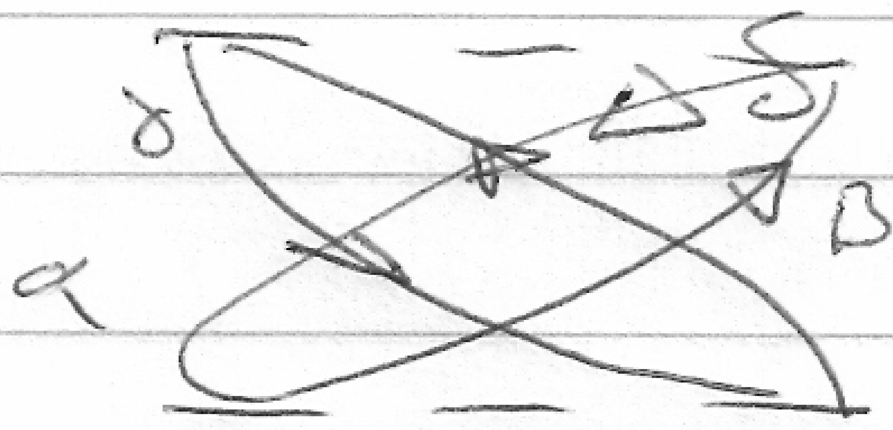
(iii)



2 holes
one loop

$-\langle \gamma\delta | v | \beta\alpha \rangle \langle \alpha\beta | v | \gamma\delta \rangle$ (−1)

(iv) $+\langle \gamma\delta | v | \beta\alpha \rangle \langle \alpha\beta | v | \delta\gamma \rangle$



2 holes
2 loops

if we had used $\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \times a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$

we get the same expressions.
In Goldstone representation
(i) = (iv) and (ii) = (iii)

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b) Diagram rules

we write now the diagram rules

① For a diagram with n H_I interactions, draw n-vertices located at times $0, t_1 \dots t_{n-1}$ ordered as

$0 > t_1 > t_2 \dots > t_{n-1}$

Each vertex can either be a a Hugenholtz antisymmetrized vertex (marked by a •) or a one body vertex U marked as

---X

② Draw all topologically distinct diagrams by linking up particle and hole lines with various vertices. Two diagrams can be made topologically equivalent by deformation of fermion lines under the restriction that

(i) The time ordering of a diagram is not altered.

(ii) Particle lines remain particle lines and idem for hole lines

(iii) The ordering at $t=0$ and $t=-\infty$ is not altered.

③ Explicit evaluation of each diagram

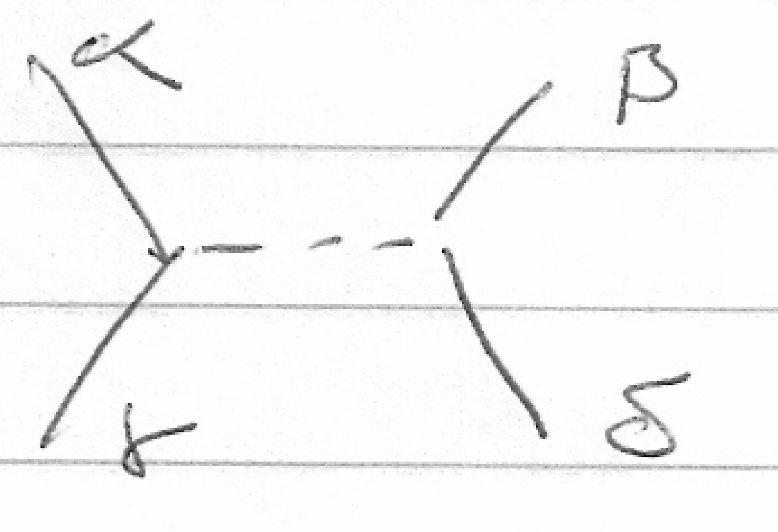
For each topologically distinct diagram

<u>3-1</u>

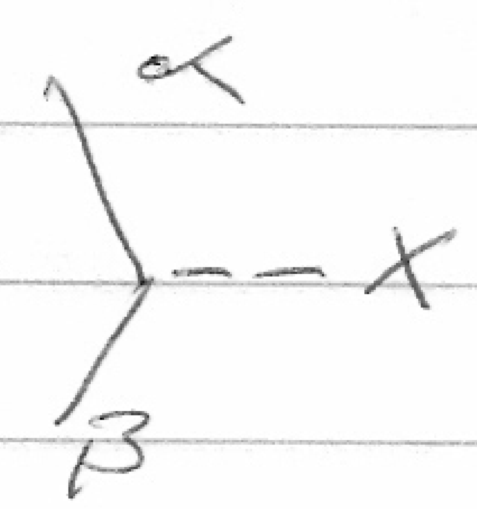
Pull open the diagram by stretching the dot vertex (•) into a dashed line vertex

- - - -

<u>3-2</u> Each vertex gives a contribution $v_{\alpha\beta\gamma\delta}$



<u>3-3</u> Each U-vertex gives a contribution $U_{\alpha\beta}$



3-4 There is a factor

$$(-1)^{n_e + n_h}$$

n_e = # number of loops
n_h = # number of hole lines

3-5 For each interval between two successive vertices (with minimum one single-particle states that is passive, that is > F) with particle lines $p_1 p_2 \ldots p_m$ and hole lines $h_1 h_2 \ldots h_m$ there is a factor

$$\frac{1}{\sum_{j=1}^{m} \varepsilon_{h_j} - \sum_{i=1}^{m} \varepsilon_{p_i}}$$

3-6 there is a factor $\left(\frac{1}{2}\right)^{n_{ep}}$

where n_{ep} = # pairs of lines that begin at the same interaction and end at the same interaction and go in the same direction

3-7 sum freely over all intermediate states

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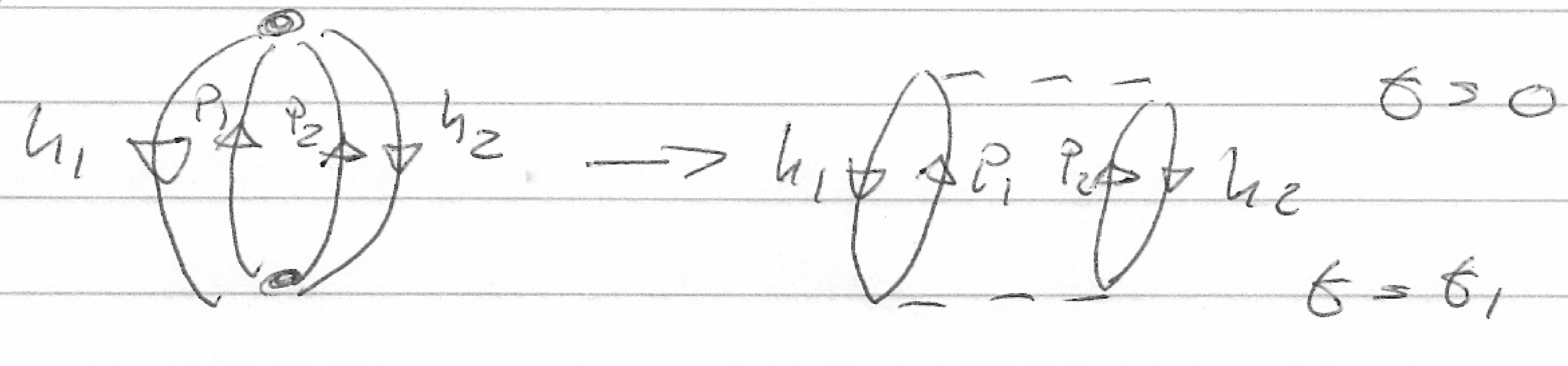
c) Examples

Here we demonstrate and also derive some of the above rules

a)



it has 2 hole lines
it has 2 loops } factor $= +1$

Energy deno $\frac{1}{\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2}}$

It has two equivalent pairs $p_1 p_2$ which begin at the same vertex and end at the same vertex $\to$ $\frac{1}{2}$ factor

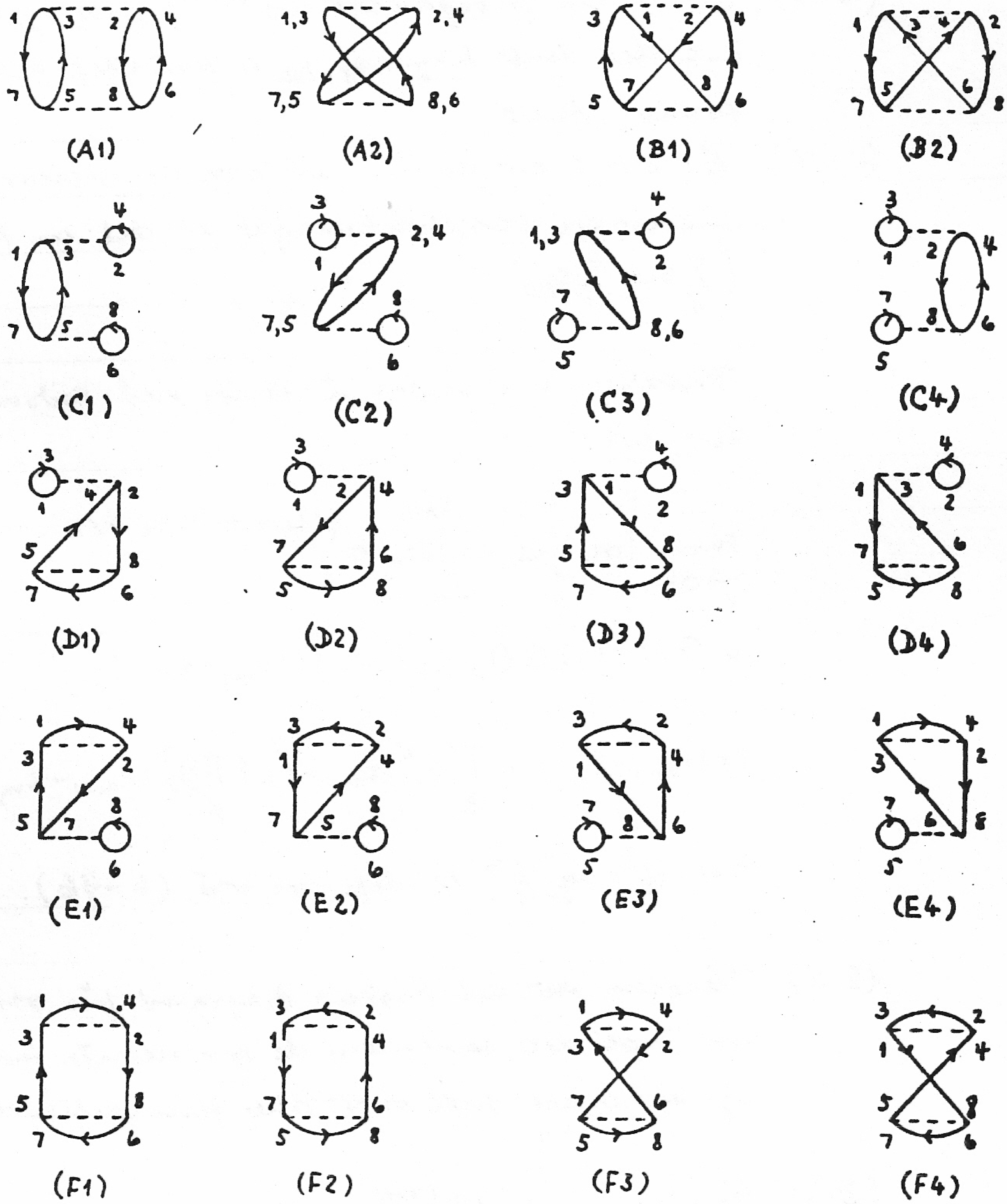
$h_1 h_2$ is also a pair $\to \frac{1}{2}$

each vertex gives either
$v_{h_1 h_2 p_1 p_2}$ or $v_{p_1 p_2 h_1 h_2}$

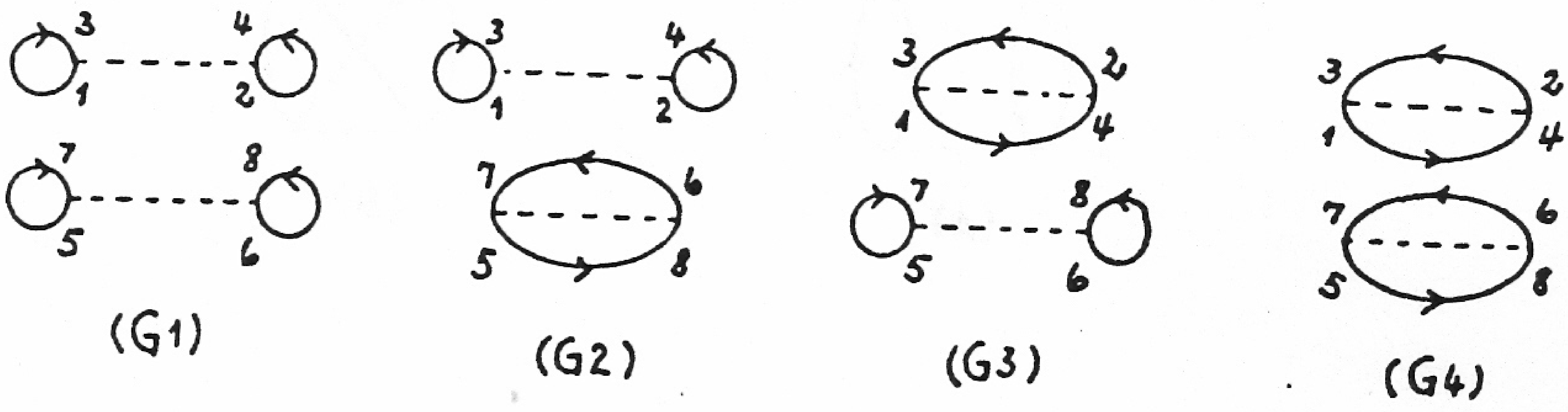
Sum freely over the states

$$\Rightarrow \frac{1}{4} \sum_{\substack{p_1 p_2 > F \\ h_1 h_2 \leq F}} \frac{|v_{h_1 h_2 p_1 p_2}|^2}{\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2}}$$

All possible diagrams to second order

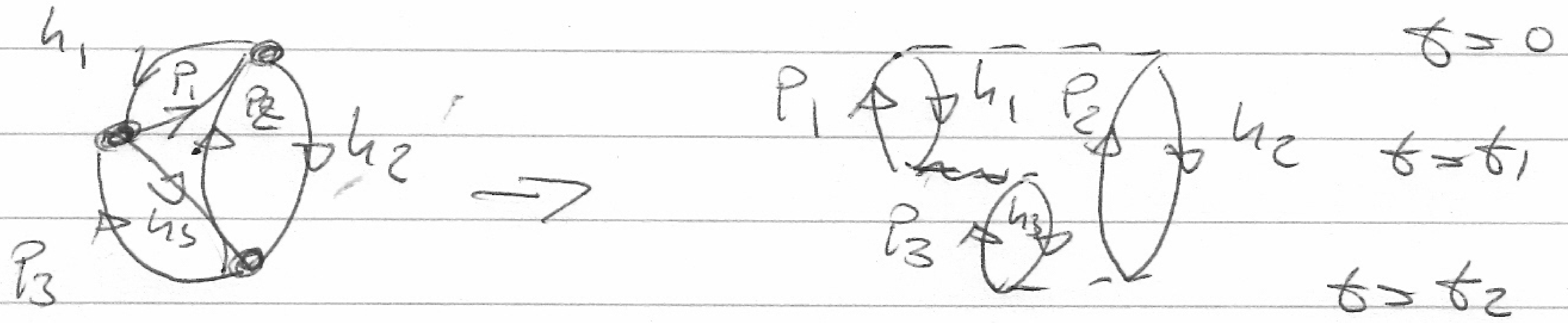


Diagrammatic representation of $\Delta E_0^{(2)}$



Unlinked second order diagrams of ΔE_0.

These diagrams are unlinked and do not arise in standard Rayleigh-Schrödinger theory, or Brillouin-Wigner theory, why ?...



$\left.\begin{array}{l} \#\text{ hole lines} = 3 \\ \#\text{ closed loops} = 3 \end{array}\right\} \quad (-1)^6 = +1$

~~# equivalent pairs = 0~~

Deno : $\dfrac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2}} \quad \dfrac{1}{\varepsilon_{h_2}+\varepsilon_{h_3}-\varepsilon_{p_3}-\varepsilon_{p_2}}$

vertices : $v_{h_1 h_2 p_1 p_2}\; v_{p_1 h_3 h_1 p_3}\; v_{p_3 p_1 h_3 h_2}$

=>

$$\sum_{\substack{p_1 p_2 p_3 > F \\ h_1 h_2 h_3 \leq F}} \frac{v_{h_1 h_2 p_1 p_2}\; v_{p_1 h_3 h_1 p_3}\; v_{p_3 p_1 h_3 h_2}}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})(\varepsilon_{h_2}+\varepsilon_{h_3}+\varepsilon_{p_3}-\varepsilon_{p_1})}$$

To see that the deno is correct, it is always useful in the beginning to carry out the time integration

$$\lim_{\varepsilon\to 0^+} \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{0} dt_1 \int_{-\infty}^{t} dt_2$$

$$\times\, e^{-i/\hbar(\varepsilon_{h_3}+\varepsilon_{h_2}-\varepsilon_{p_3}-\varepsilon_{p_2}+i\varepsilon)t_2}$$

$$\times\, e^{-i/\hbar(\varepsilon_{h_1}+\varepsilon_{p_3}-\varepsilon_{p_1}-\varepsilon_{h_3})t_1}$$

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$$= \lim_{\varepsilon \to 0^+} \left(\frac{-i}{\hbar}\right) \int_{-\infty}^{0} dt_1$$

~~$\times\, e^{-i/\hbar\,(\varepsilon_{h_3} + \varepsilon_{h_2} + \varepsilon_{h_1} - \varepsilon_{p_1} - \varepsilon_{p_2}}$~~

$$\times\, e^{-i/\hbar\,(\varepsilon_{h_1} + \varepsilon_{p_3} - \varepsilon_{p_1} - \varepsilon_{h_3} + \varepsilon_{h_2} + \varepsilon_{h_3} - \varepsilon_{p_2} - \varepsilon_{p_3})\, t_1}$$

$$\times\, e^{-i/\hbar\,(2i\varepsilon)\, t_1} \times \frac{1}{(i\varepsilon + \varepsilon_{h_3} + \varepsilon_{h_2} - \varepsilon_{p_3} - \varepsilon_{p_2})}$$

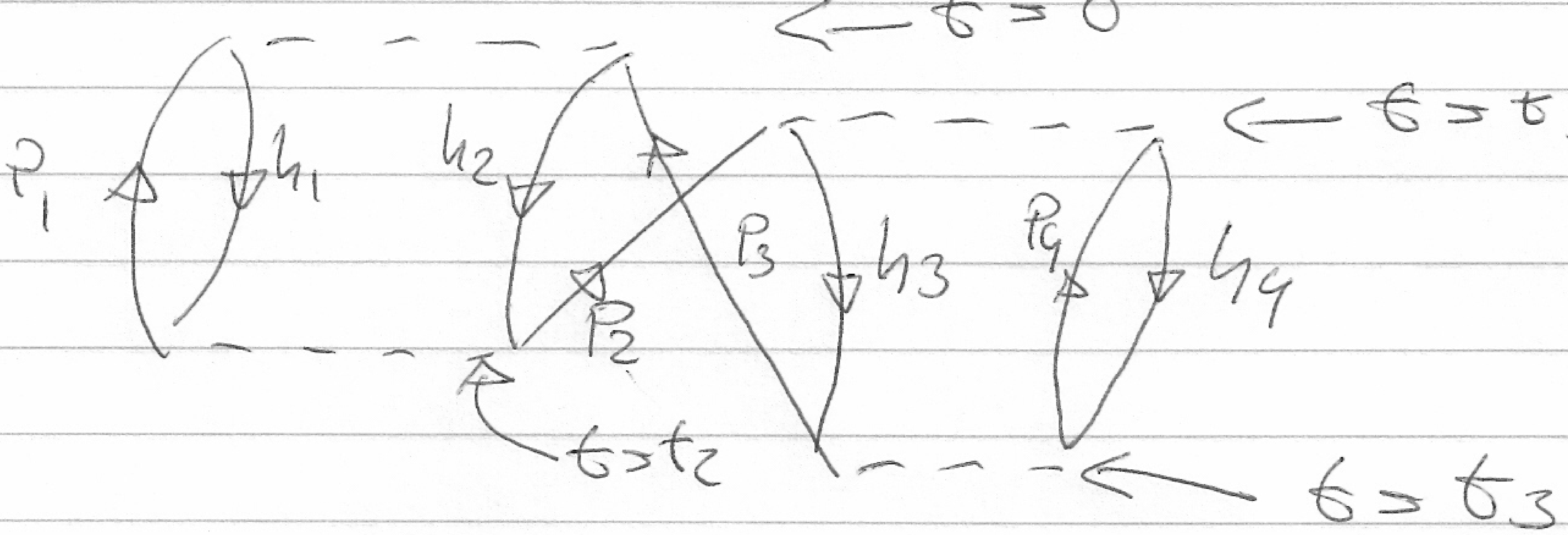
$$= \lim_{\varepsilon \to 0^+} \frac{1}{(\varepsilon_{h_3} + \varepsilon_{h_2} - \varepsilon_{p_3} - \varepsilon_{p_2} + i\varepsilon)}$$

$$\times \frac{1}{(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2} + 2i\varepsilon)}$$

$$= \frac{1}{\varepsilon_{h_3} + \varepsilon_{h_2} - \varepsilon_{p_3} - \varepsilon_{p_2}} \; \frac{1}{\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2}}$$

A subtle point

We stated that we sum freely over all single-particle states. This means that we can violate the Pauli principle. Consider the following case (we have opened up all vertices)



The expression is

\# holes = 4

\# loops = 3

\# equivalent pairs = 2 $(h_1 h_2)$ $(h_3 h_4)$

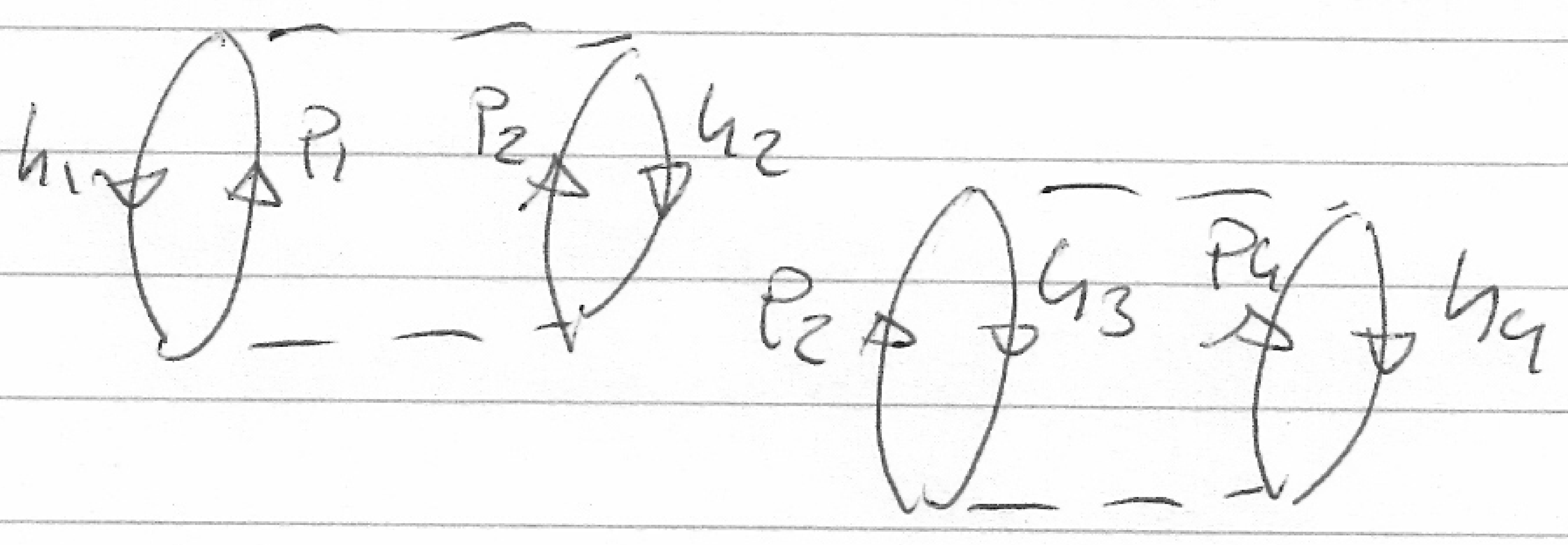
$$-\frac{1}{4}\sum_{\substack{p_1p_2p_3p_4>F\\ h_1h_2h_3h_4\le F}} \frac{1}{\varepsilon_{h_3}+\varepsilon_{h_4}-\varepsilon_{p_3}-\varepsilon_{p_4}}$$

$$\times\frac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}+\varepsilon_{h_3}+\varepsilon_{h_4}-\varepsilon_{p_1}-\varepsilon_{p_2}-\varepsilon_{p_3}-\varepsilon_{p_4}}$$

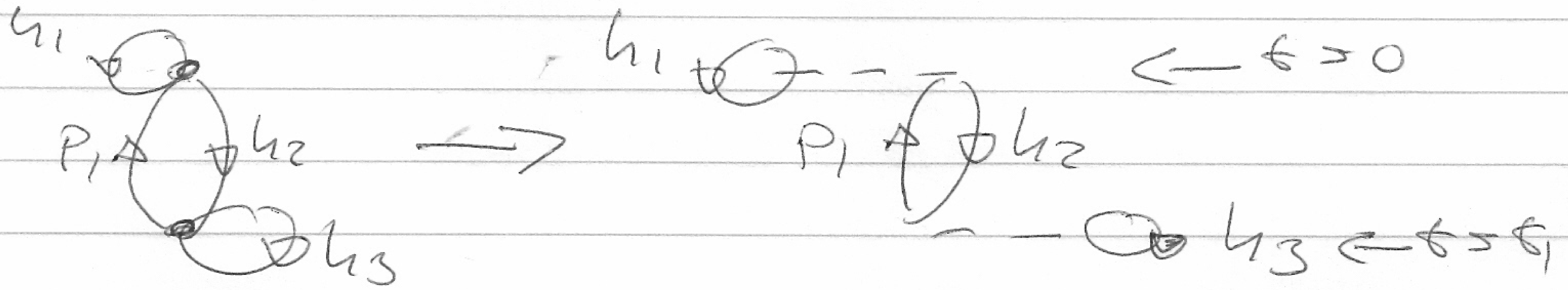
$$\times \frac{1}{\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_3}}$$

$$\times\ V_{h_1 h_2 p_1 p_3} V_{h_3 h_4 p_2 p_4} V_{h_1 h_2 p_1 p_2} V_{p_3 p_4 h_3 h_4}$$

we can have a case where $p_3 = p_2$ since we are summing freely over all quantum numbers. Such a contribution violates the Pauli principle but is cancelled exactly by the unlinked diagram



This diagram is contained in the denominator and the numerator and cancel each other. We must therefore keep the Pauli principle violating diagram.



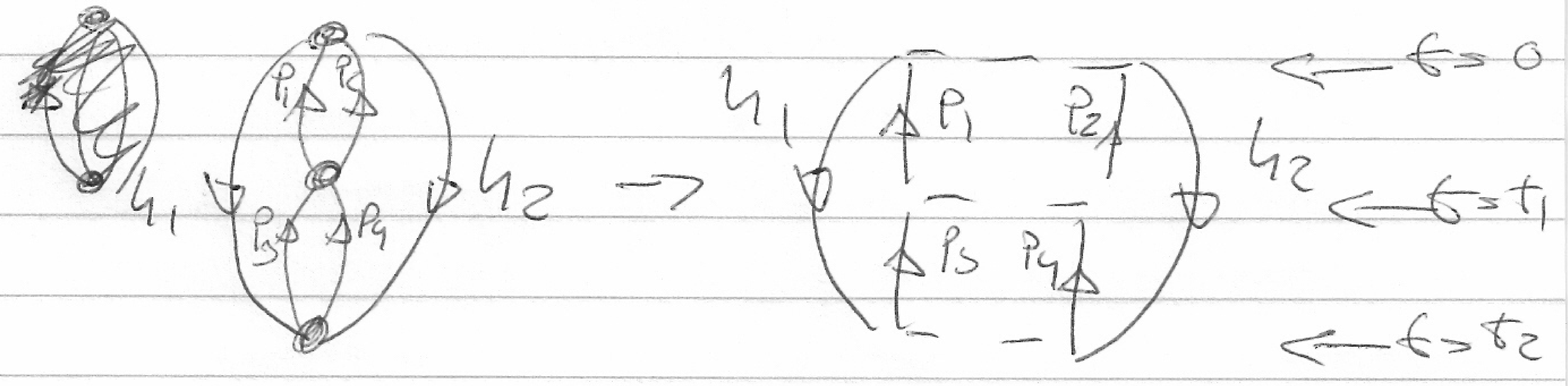
\# hole lines = 3

\# loops = 3

Deno = $\dfrac{1}{\varepsilon_{h_2} - \varepsilon_{p_1}}$

\# equivalent pairs = 0

$$\Rightarrow \sum_{\substack{h_1 h_2 h_3 \\ p_1}} \frac{v_{h_1 h_2 h_1 p_1} \, v_{p_1 h_3 h_2 h_3}}{\varepsilon_{h_2} - \varepsilon_{p_1}}$$



\# hole lines = 2 \
\# loops = 2 } $(-1)^4 = +1$

\# equivalent pairs = 3

Deno $= \frac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_3}-\varepsilon_{p_4}} \frac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2}}$

$$\Rightarrow \frac{1}{8} \sum_{\substack{p_1 p_2 p_3 p_4 > F \\ h_1 h_2 \leq F}} \frac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_3}-\varepsilon_{p_4}} \frac{1}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2}}$$

$$\times\ \overline{v}_{h_1 h_2 p_1 p_2}\ \overline{v}_{p_1 p_2 p_3 p_4}\ \overline{v}_{p_3 p_4 h_1 h_2}$$