Lecture FYS4480/9480, November 15, 2024

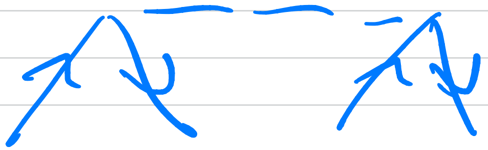
Linked and unlinked diagrams

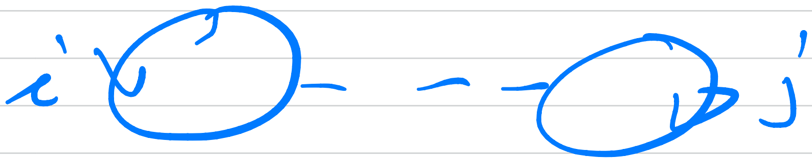
$$|\psi^{(2)}\rangle =$$

$$\sum_{MN} \frac{|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_N\rangle\langle\Phi_N|H_1|\Phi_0\rangle}{(E_0-E_M)(E_0-E_N)}$$

$$-\left\{\sum_M \frac{|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_0\rangle}{(E_0-E_M)^2}\right\}$$

$$\times\langle\Phi_0|H_1|\Phi_0\rangle$$

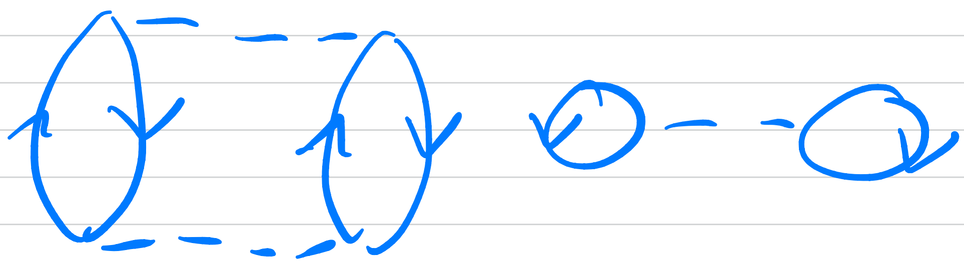




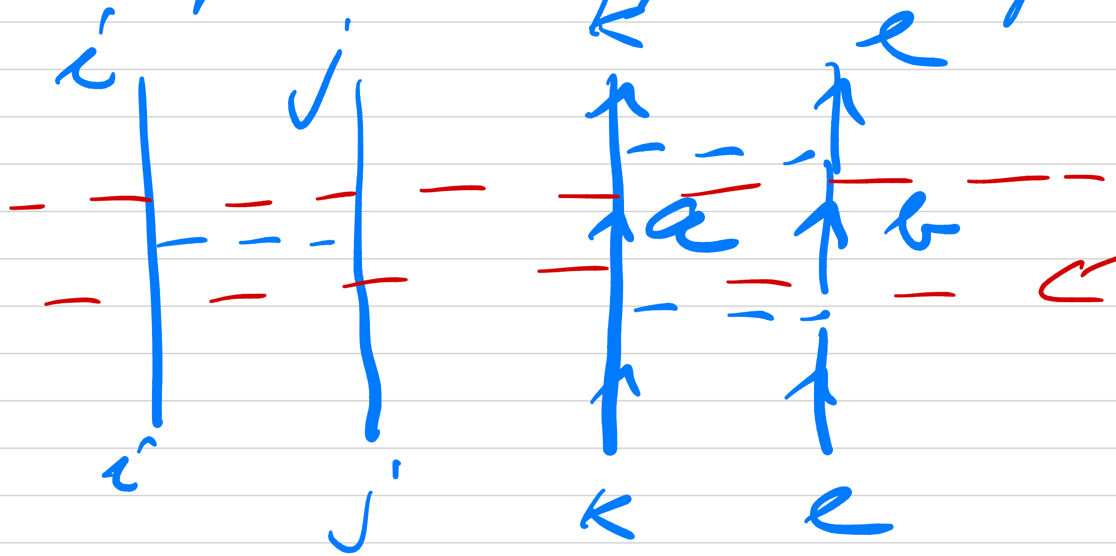
$$\langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$\langle \Phi_0 | H_1$$

unlinked



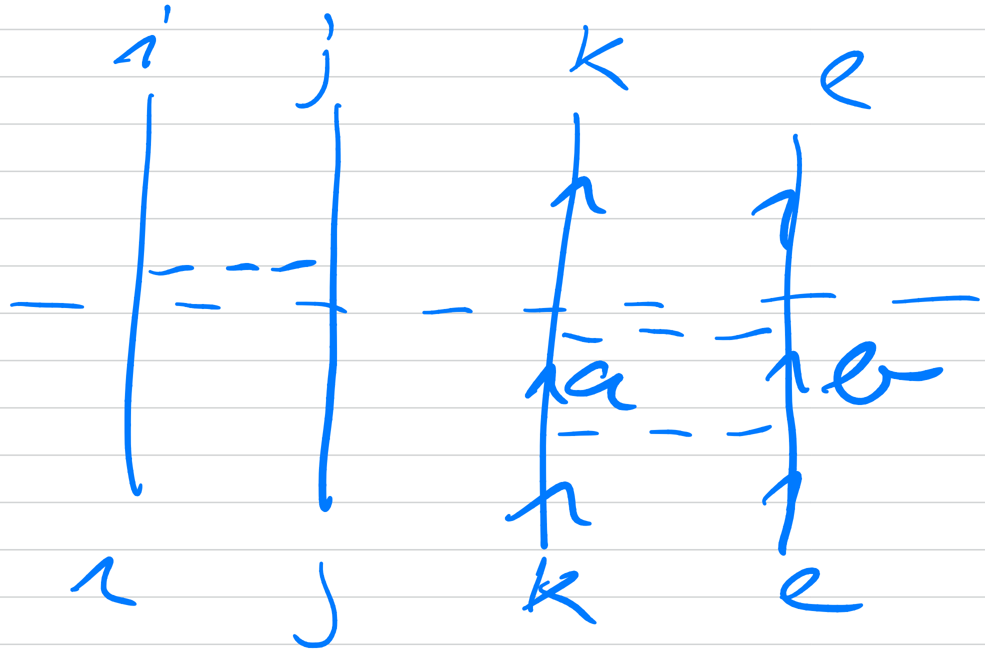
Open up in particle formalism



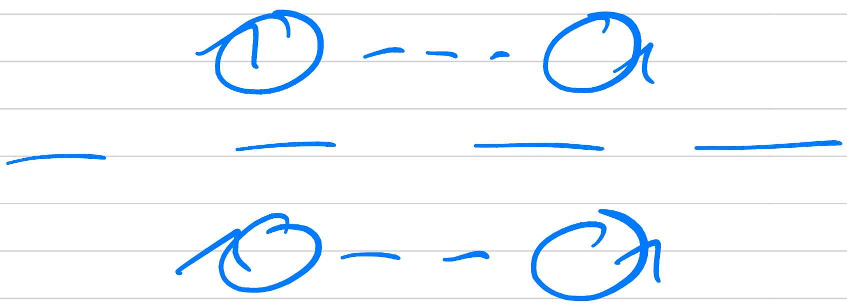
within $Q = \sum |\Phi_M\rangle$

$M>0$

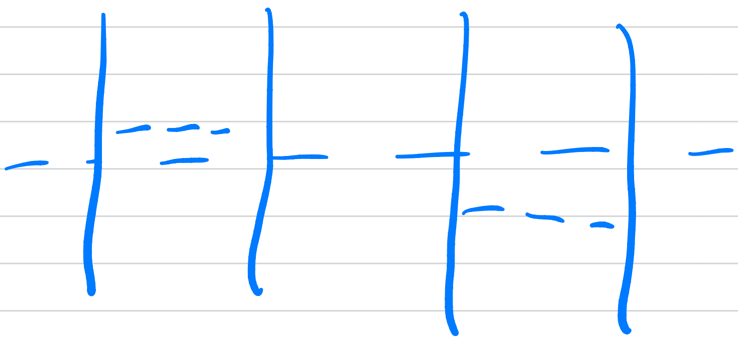
$\times \langle \Phi_M|$



$\in |\Phi_0\rangle$



$\in |\Phi_0\rangle$

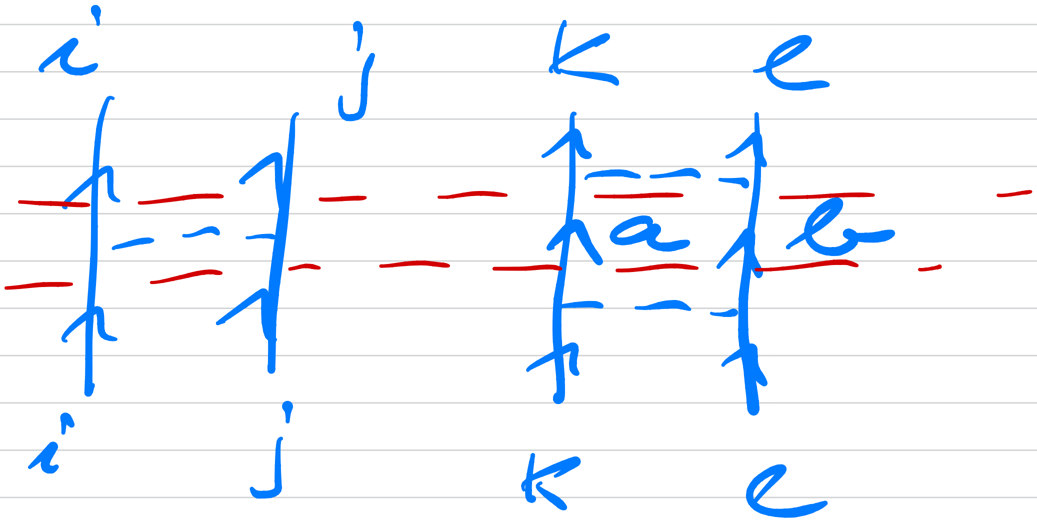


$\in |\Phi_0\rangle$ not allowed

$$\Delta E_0^{(3)} = \langle \Phi_0 | \hat{H}_1 \underbrace{\frac{\hat{Q}}{\hat{e}_0}}_{\hat{R}} \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 | \Phi_0 \rangle$$

$$- \langle \Phi_0 | H_1 \left(\frac{\hat{Q}}{e_0} \right)^2 H_1 | \Phi_0 \rangle \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

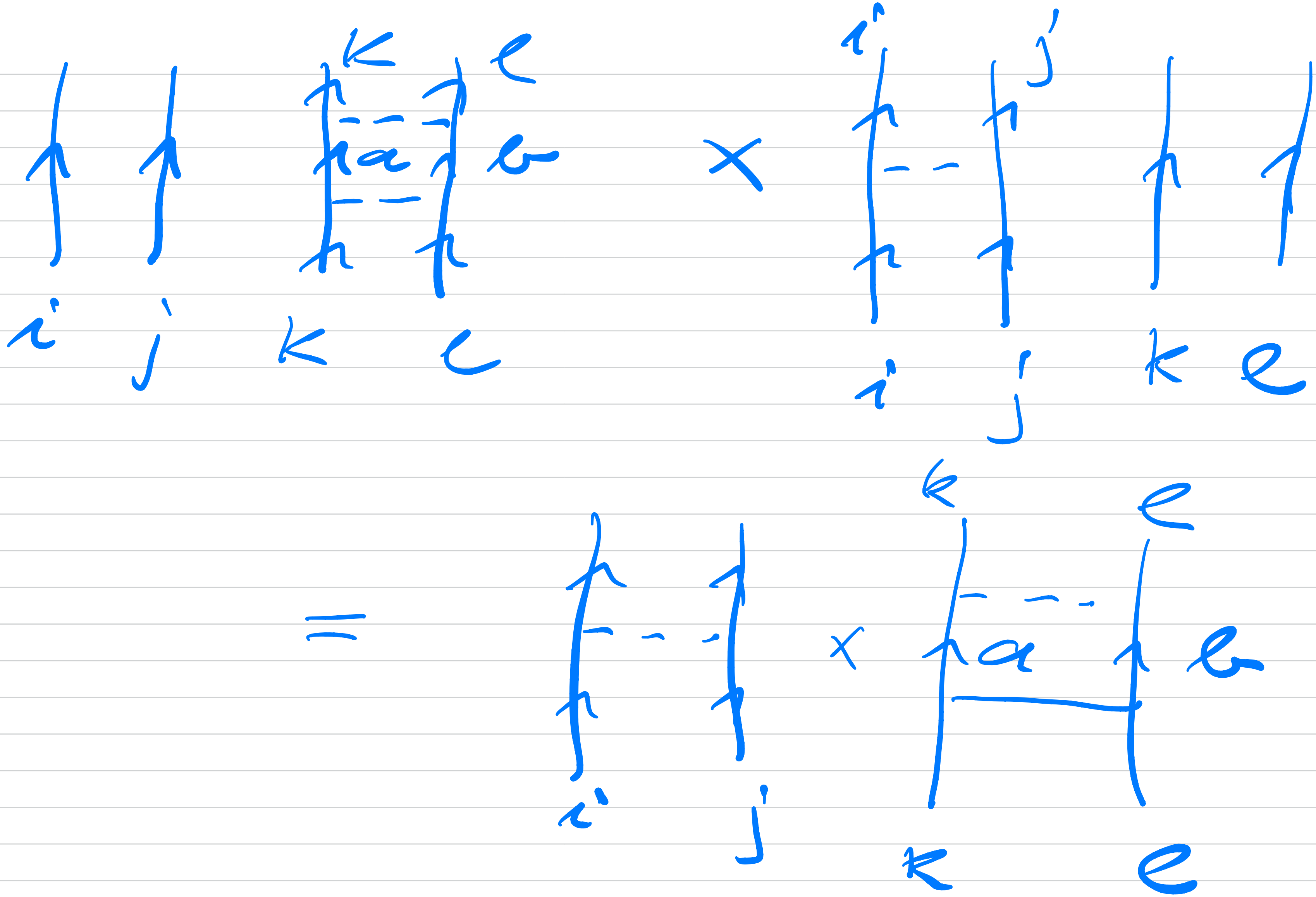
case with four particles unlinked



(could arise from first term in $\Delta E^{(3)}$)

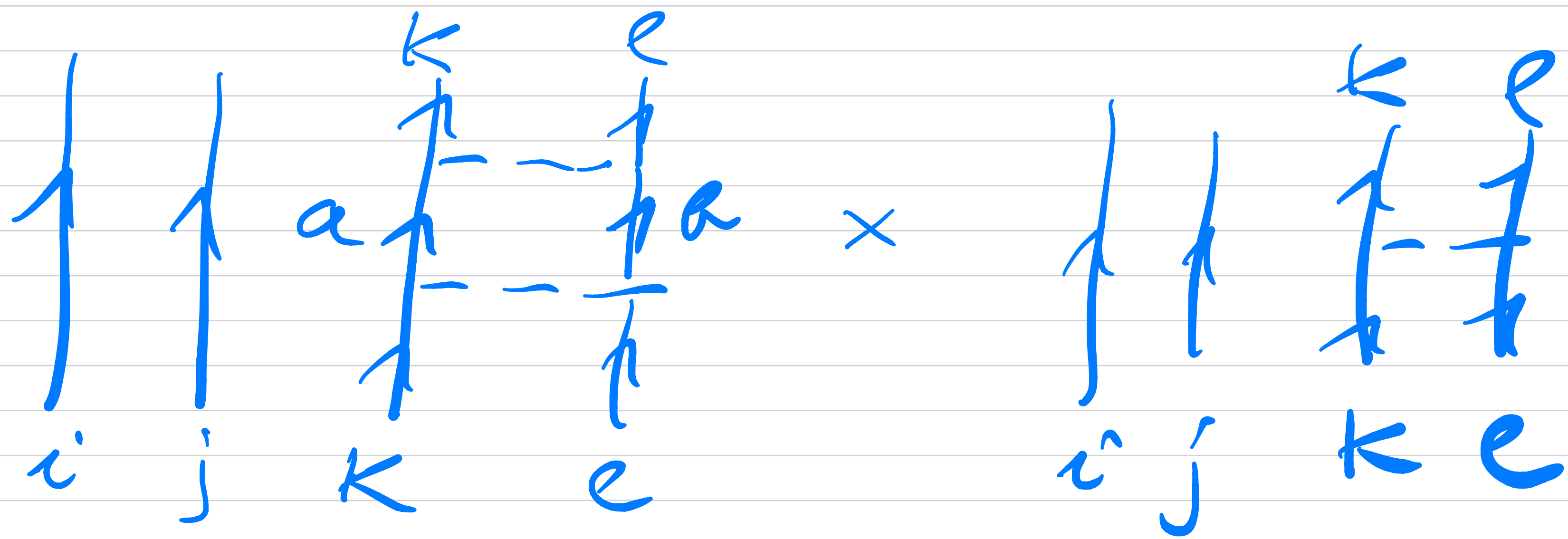
$$\frac{\langle kl|v|ab\rangle\langle ij|v|ij\rangle\langle ab|v|kl\rangle}{(\varepsilon_k+\varepsilon_l-\varepsilon_a-\varepsilon_b)^2}$$

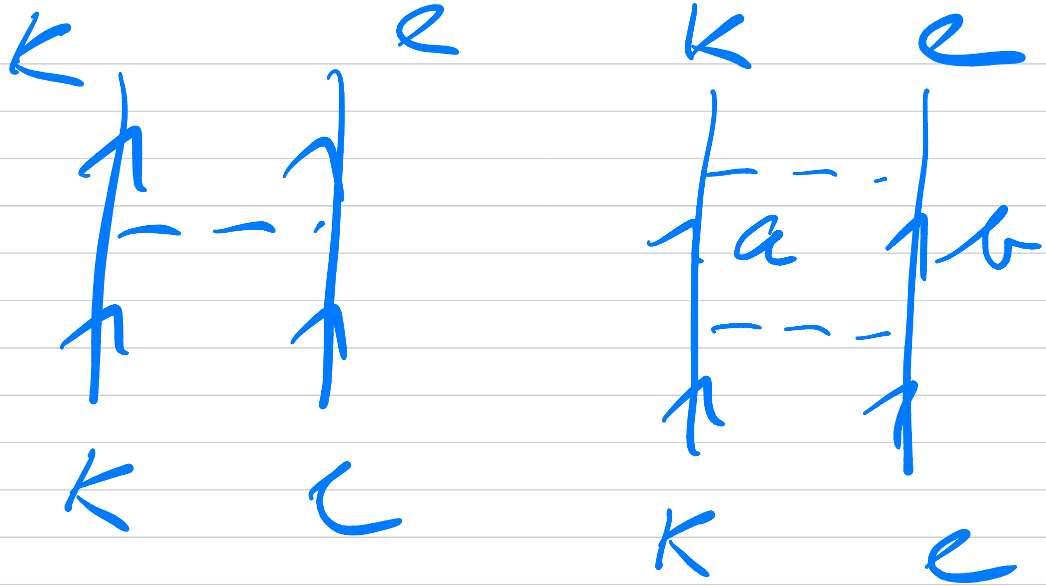
Gets cancelled from



k e a b
i j k e
i j
i j k e
k e
a b
i j k e

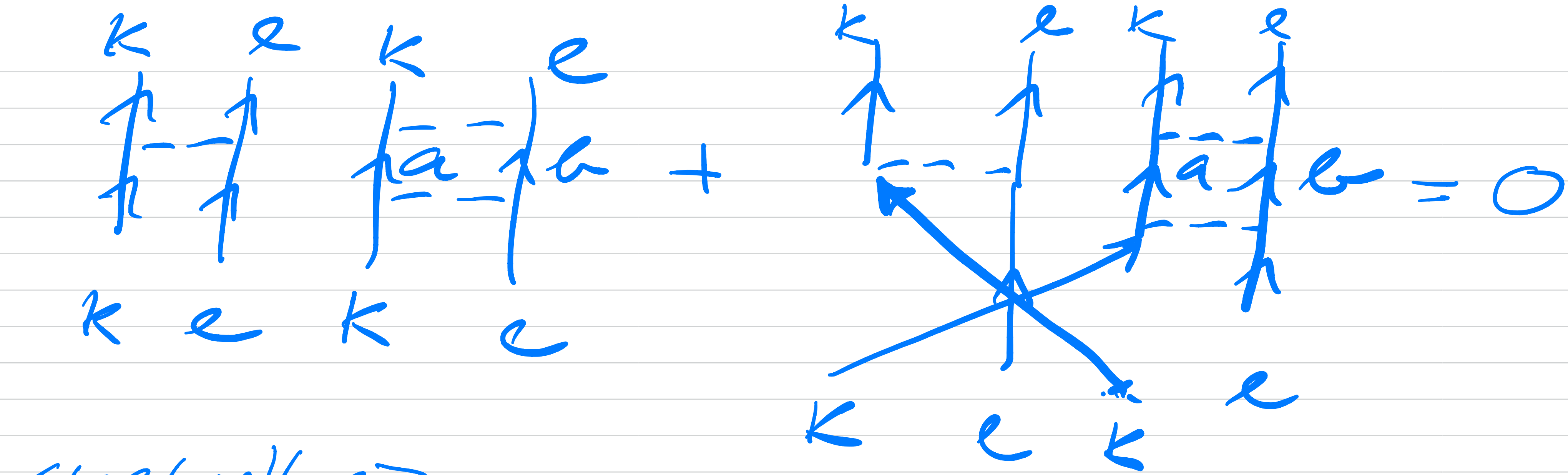
There are however additional terms from the second $\Delta E^{(3)}$ term that are unlinked but do not get cancelled by the first term,



$=$ 

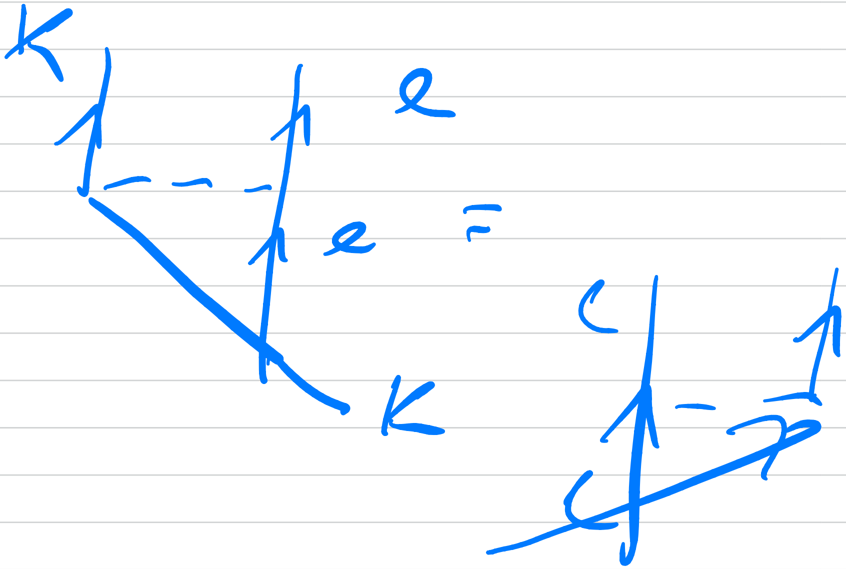
Breaks Pauli principle

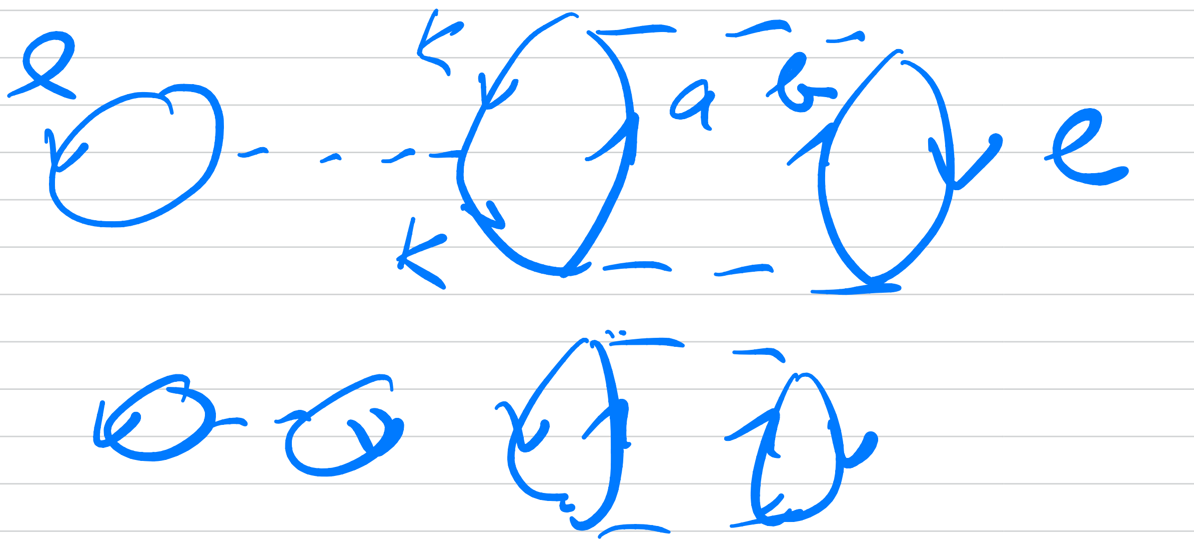
if we include this diagram with its exchange diagram in the first term of $\Delta E_0^{(3)}$



$\langle ke|v|ke\rangle$
$= \langle ek|v|ek\rangle$

linked





Linked diagram theorem

(quasi proof + more discussions in Shavitt & Bartlett chapter 6)

Retain only linked diagrams including those that break the Pauli principle

$$\hat{R} = \frac{\hat{Q}}{e_0} = \frac{\hat{Q}}{\mathcal{E}_0 - \hat{H}_0}$$

$$\Delta E_0^{(n)} = \langle \Phi_0 | \hat{H}_1 (\hat{R} H_1)^{n-1} | \Phi_0 \rangle$$

Let us go back to simple example

E_2 ——

E_1 ——

$$H_0 |\Phi_1\rangle = \varepsilon_1 |\Phi_1\rangle$$

$$H_0 |\Phi_2\rangle = \varepsilon_2 |\Phi_2\rangle$$

$$\det \begin{bmatrix} \varepsilon_1 - E_1 & \lambda \\ \lambda & \varepsilon_2 - E_2 \end{bmatrix} = 0$$

$$\langle \Phi_i | H_1 | \Phi_i \rangle = 0$$

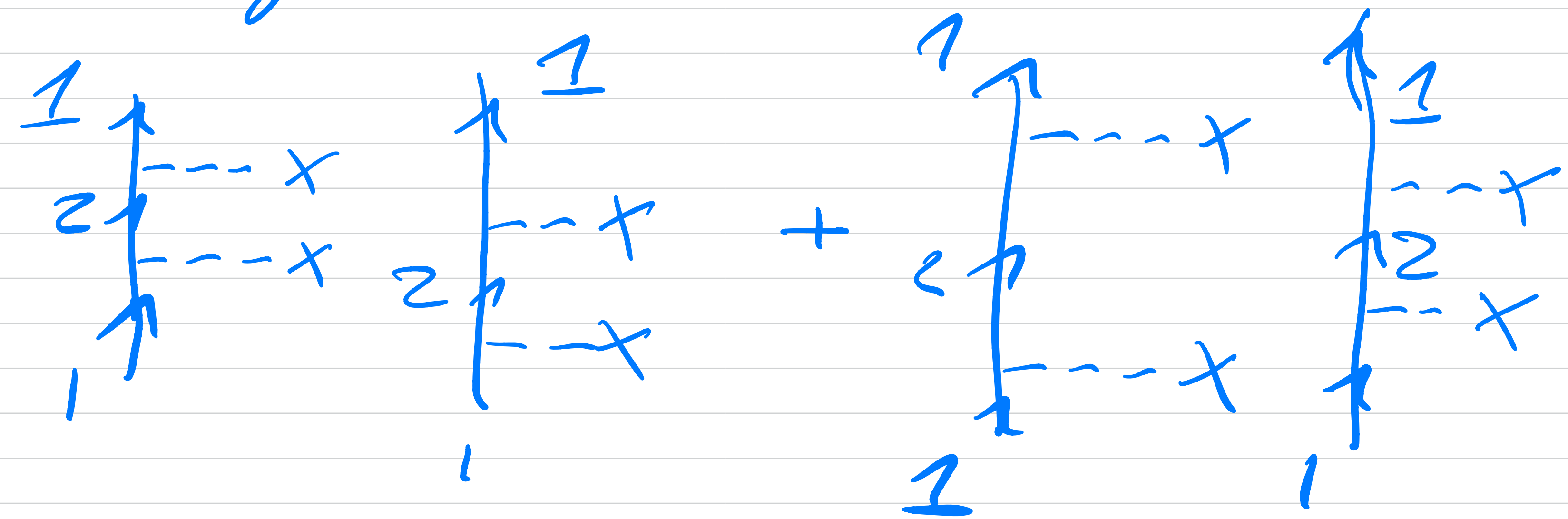
$$\langle \Phi_1 | H_1 | \Phi_2 \rangle = \lambda$$

$$
\begin{aligned}
\Delta E_1^{(4)} = & \langle \hat{H}_1 \hat{R} \hat{H}_1 \hat{R} \hat{H}_1 \hat{R} H_1 \rangle \\
& - \langle \hat{H}_1 \hat{R} \langle H_1 \rangle \hat{R} \hat{H}_1 \hat{R} H_1 \rangle \\
& - \langle \hat{H}_1 \hat{R} \hat{H}_1 \hat{R} \langle \hat{H}_1 \rangle \hat{R} H_1 \rangle \\
& + \langle \hat{H}_1 \hat{R} \langle H_1 \rangle \hat{R} \langle H_1 \rangle \hat{R} \hat{H}_1 \rangle \\
& - \langle \hat{H}_1 \hat{R} \langle \hat{H}_1 \hat{R} H_1 \rangle \hat{R} H_1 \rangle
\end{aligned}
$$

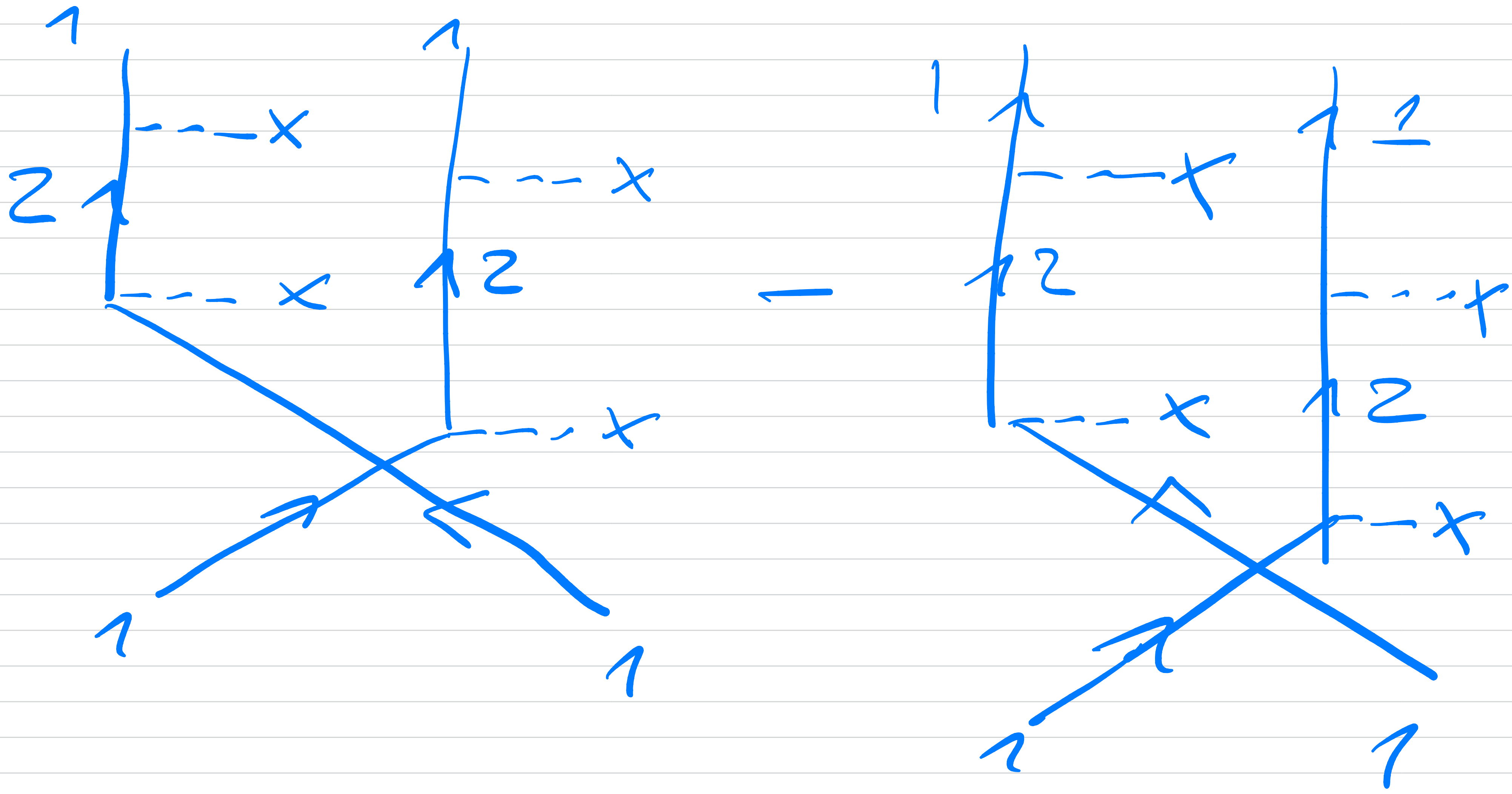
$$
\begin{aligned}
\Delta E_1^{(4)} = & - \langle \phi_1 | \hat{H}_1 | \phi_2 \rangle \langle \Phi_2 | \hat{H}_1 | \phi_1 \rangle \\
& \times \langle \phi_1 | \hat{H}_1 | \phi_2 \rangle \langle \phi_2 | \hat{H}_1 | \phi_1 \rangle \\
& \times \frac{1}{(\varepsilon_1 - \varepsilon_2)^3}
\end{aligned}
$$

$$= -\frac{\lambda^4}{(\varepsilon_1-\varepsilon_2)^3}$$

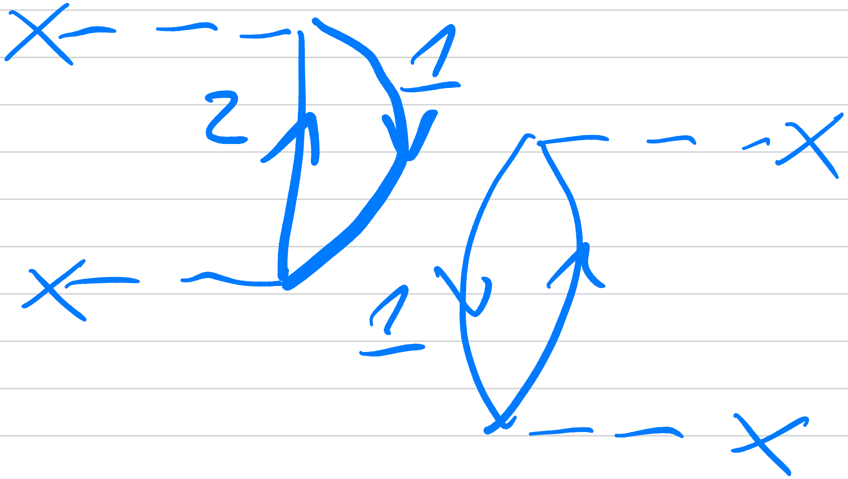
Diagrammatic analysis



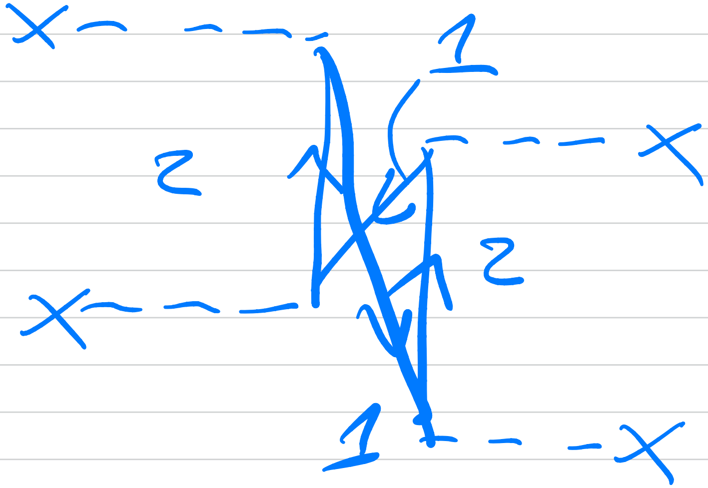
Add and subtract



$= 0$



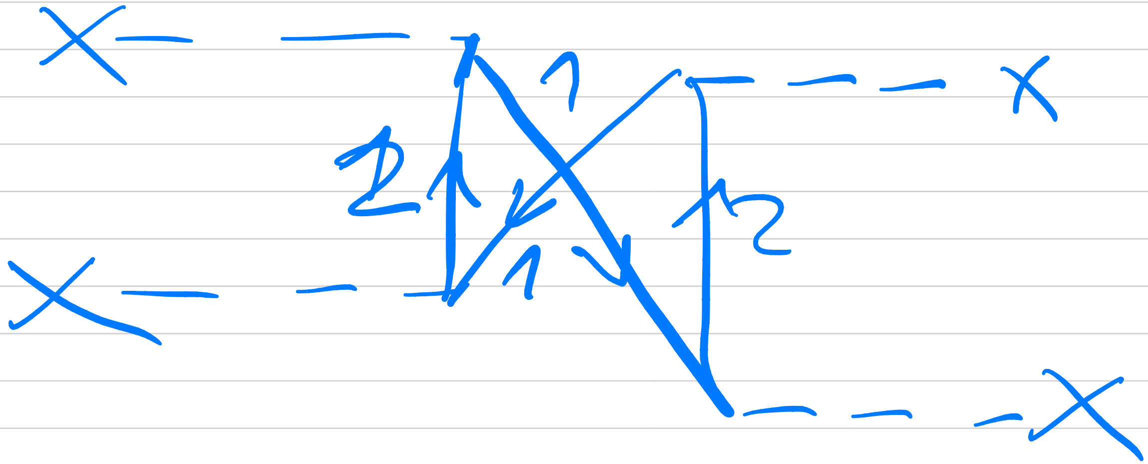
+



unlinked
Pauli
violating

linked
Pauli
violating
diagram

left with



$$= -\frac{x^4}{(\varepsilon_1 - \varepsilon_2)^3}$$

Physical interpretations of unlinked diagrams

size extensivity of Energy

$E \sim N$

electron gas

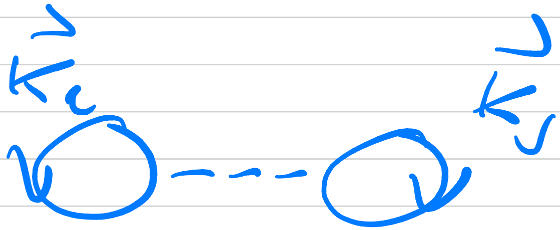
$$\langle \vec{k}_l \vec{k}_j | v | \vec{k}_m \vec{k}_n \rangle$$

$$= \delta_{\vec{k}_l+\vec{k}_j,\, \vec{k}_m+\vec{k}_n} \times \frac{1}{V}$$

$$\times \int v(\vec{r}_{12})\, d\vec{r}_{12}\, e^{i(\vec{k}_l-\vec{k}_j)\vec{r}_{12}}$$

$$\langle \vec{k}_i \vec{k}_j | V | \vec{k}_m \vec{k}_n \rangle \propto \frac{1}{V}$$

$$\Delta E_0^{(1)} =$$



$$= \frac{1}{2} \sum_{\vec{k}_i \vec{k}_j \le \vec{k}_F} \langle \vec{k}_i \vec{k}_j | v | \vec{k}_i \vec{k}_j \rangle$$

$$\sum_{k} \rightarrow \frac{V}{(2\pi)^3} \int d\vec{k}$$

$$\frac{V}{(2\pi)^3} \int_0^{\vec{k}_F} d\vec{k} = N \qquad \rho = \frac{N}{V}$$

$$\Delta E_0^{(1)} = \frac{1}{2} \underbrace{\frac{V}{(2\pi)^3}\int^{k_F} d\vec{k}_1}_{c} \underbrace{\frac{V}{(2\pi)^3}\int^{k_F} d\vec{k}_j}_{c}$$

$$\times \frac{1}{V} \underbrace{\int d\vec{r}_{12}\, V(r_{12})}_{\text{constant}}$$

$$\propto N^2/V = N\rho$$

$$\frac{\Delta E_0^{(1)}}{N} \propto \rho$$

2nd-order

$\Delta E_0^{(2)} =$

$$= \frac{1}{4} \sum_{\substack{\vec{k}_{i'} \vec{k}_{j'} \\ \vec{k}_a \vec{k}_b}} \frac{|\langle \vec{k}_{i'} \vec{k}_{j'} | v | \vec{k}_a \vec{k}_b \rangle|^2}{\varepsilon_{k_{i'}} + \varepsilon_{k_{j'}} - \varepsilon_{k_a} - \varepsilon_{k_b}}$$

$$\vec{k}_a = \vec{k}_i + \vec{k}_j - \vec{k}_b$$

$$\Delta E_0^{(2)} = \frac{1}{4} \frac{V}{(2\pi)^3} \int_0^{\vec{k}_F} d\vec{k}_1 \frac{V}{(2\pi)^3} \int_0^{\vec{k}_F} d\vec{k}_j$$

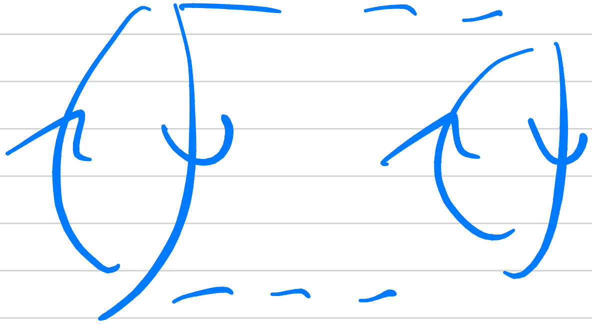
$$\times \frac{V}{(2\pi)^3} \int_{k_F}^{\infty} d\vec{k}_a \frac{|\langle \vec{k}_1 \vec{k}_j | v | \vec{k}_a k_1 + k_j - k_a \rangle|}{(\varepsilon_{k_1'} + \varepsilon_{k_j'} - \varepsilon_{k_a} - \varepsilon_{k_1 + k_j - k_a})}$$

each $\langle |v| \rangle \sim \frac{1}{V}$

$$\Delta E_0^{(2)} \sim N^2/V = N\rho$$

Third-order:

$N\rho$

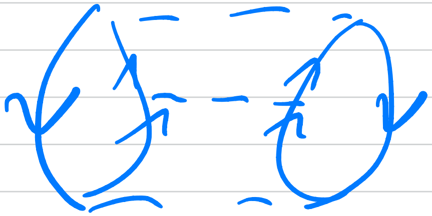


$N\rho$

unlinked

$$\Delta E_0^{(3)} = N^2\rho^2$$

unphysical dependence

 $\sim N\rho$

Coupled cluster theory

$$\langle 0p0h | H | 1p1h \rangle = 0$$

$$\langle 0p0h | H | 2p2h \rangle = 0$$

$$
\begin{array}{cccccc}
0p0h & 1p1h & 2p2h & 3p3h & \cdots & \\
\end{array}
$$

$$
\begin{bmatrix}
\times & \times & \times & 0 & 0 & \cdots \\
\times & \times & \times & \times & 0 & \cdots \\
\times & \times & \times & & & \\
0 & \times & \times & & & \\
\vdots & & \times & & & \\
\vdots & 0 & \times & & &
\end{bmatrix}
$$