

Third order onebody diagrams

Abstract

All diagrams to third order in the interaction for an arbitrary two-body interaction \hat{v} .

EXPRESSIONS

The states pq represent outgoing single-particle states. They can be either hole or particle states. Holes states are labeled as $ijk\dots$ and particle states are $abc\dots$, the standard quantum chemistry notation.

Diagram 1-5

$$\frac{1}{4} \sum_{abcd} \sum_i \frac{\langle pi|\hat{v}|ab\rangle \langle ab|\hat{v}|cd\rangle \langle cd|\hat{v}|qi\rangle}{(\varepsilon_q + \varepsilon_i - \varepsilon_c - \varepsilon_d)(\varepsilon_q + \varepsilon_i - \varepsilon_a - \varepsilon_b)}.$$

Diagram 1-6

$$-\frac{1}{4} \sum_{abc} \sum_{ij} \frac{\langle pc|\hat{v}|ab\rangle \langle ab|\hat{v}|ij\rangle \langle ij|\hat{v}|cq\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_i + \varepsilon_j - \varepsilon_p - \varepsilon_c)}.$$

Diagram 1-7

$$\frac{1}{4} \sum_{abc} \sum_{ij} \frac{\langle pc|\hat{v}|ij\rangle \langle ij|\hat{v}|ab\rangle \langle ab|\hat{v}|cq\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_p - \varepsilon_c)(\varepsilon_i + \varepsilon_j + \varepsilon_q - \varepsilon_a - \varepsilon_p - \varepsilon_b)}.$$

Diagram 1-8

$$-\frac{1}{4} \sum_a \sum_{ijkl} \frac{\langle ij|\hat{v}|qa\rangle \langle kl|\hat{v}|ij\rangle \langle pa|\hat{v}|kl\rangle}{(\varepsilon_k + \varepsilon_l - \varepsilon_p - \varepsilon_a)(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_p)}.$$

Diagram 1-9

$$-\frac{1}{4} \sum_{ab} \sum_{ijk} \frac{\langle jp|\hat{v}|ab\rangle \langle ab|\hat{v}|ik\rangle \langle ik|\hat{v}|qj\rangle}{(\varepsilon_k + \varepsilon_i - \varepsilon_a - \varepsilon_b)(\varepsilon_q + \varepsilon_j - \varepsilon_a - \varepsilon_b)}.$$

Diagram 1-10

$$-\frac{1}{4} \sum_{ab} \sum_{ijk} \frac{\langle ab|\hat{v}|qk\rangle \langle kp|\hat{v}|ij\rangle \langle ij|\hat{v}|ab\rangle}{(\varepsilon_k + \varepsilon_q - \varepsilon_a - \varepsilon_b)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-11

$$-\frac{1}{2} \sum_{ab} \sum_{ijk} \frac{\langle ab|\hat{v}|kj\rangle \langle pk|\hat{v}|qi\rangle \langle ij|\hat{v}|ab\rangle}{(\varepsilon_k + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-12

$$\frac{1}{2} \sum_{abc} \sum_{ij} \frac{\langle cb|\hat{v}|ij\rangle \langle ij|\hat{v}|ab\rangle \langle pa|\hat{v}|qc\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_c)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-13

$$\frac{1}{2} \sum_{abc} \sum_{ij} \frac{\langle ab|\hat{v}|ij\rangle \langle ic|\hat{v}|ab\rangle \langle jp|\hat{v}|cq\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_j - \varepsilon_c)}.$$

Diagram 1-14

$$\frac{1}{2} \sum_{abc} \sum_{ij} \frac{\langle pc|\hat{v}|qi\rangle \langle ab|\hat{v}|cj\rangle \langle ij|\hat{v}|ab\rangle}{(\varepsilon_i + \varepsilon_q - \varepsilon_p - \varepsilon_c)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-15

$$-\frac{1}{2} \sum_{ab} \sum_{ijk} \frac{\langle kp|\hat{v}|bq\rangle \langle ij|\hat{v}|ak\rangle \langle ab|\hat{v}|ij\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_k - \varepsilon_b)}.$$

Diagram 1-16

$$-\frac{1}{2} \sum_{ab} \sum_{ijk} \frac{\langle pa|\hat{v}|qk\rangle \langle kb|\hat{v}|ij\rangle \langle ij|\hat{v}|ab\rangle}{(\varepsilon_q + \varepsilon_k - \varepsilon_p - \varepsilon_a)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-17

$$\sum_{abc} \sum_{ij} \frac{\langle ac|\hat{v}|ij\rangle \langle jb|\hat{v}|cq\rangle \langle ip|\hat{v}|ab\rangle}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_c)(\varepsilon_q + \varepsilon_i - \varepsilon_a - \varepsilon_b)}.$$

Diagram 1-18

$$\sum_{abc} \sum_{ij} \frac{\langle ij|\hat{v}|ab\rangle \langle bp|\hat{v}|jc\rangle \langle ac|\hat{v}|iq\rangle}{(\varepsilon_i + \varepsilon_q - \varepsilon_a - \varepsilon_c)(\varepsilon_q + \varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_p)}.$$

Diagram 1-19

$$\sum_{abc} \sum_{ij} \frac{\langle pi|\hat{v}|ab\rangle \langle jb|\hat{v}|ci\rangle \langle ac|\hat{v}|qj\rangle}{(\varepsilon_q + \varepsilon_j - \varepsilon_a - \varepsilon_c)(\varepsilon_q + \varepsilon_i - \varepsilon_a - \varepsilon_b)}.$$

Diagram 1-20

$$-\sum_{ab} \sum_{ijk} \frac{\langle pb|\hat{v}|ik\rangle \langle ka|\hat{v}|bj\rangle \langle ij|\hat{v}|qa\rangle}{(\varepsilon_i + \varepsilon_k - \varepsilon_p - \varepsilon_b)(\varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_p)}.$$

Diagram 1-21

$$-\sum_{ab} \sum_{ijk} \frac{\langle ij|\hat{v}|aq\rangle \langle kp|\hat{v}|bj\rangle \langle ab|\hat{v}|ik\rangle}{(\varepsilon_i + \varepsilon_k - \varepsilon_a - \varepsilon_b)(\varepsilon_j + \varepsilon_i - \varepsilon_a - \varepsilon_p)}.$$

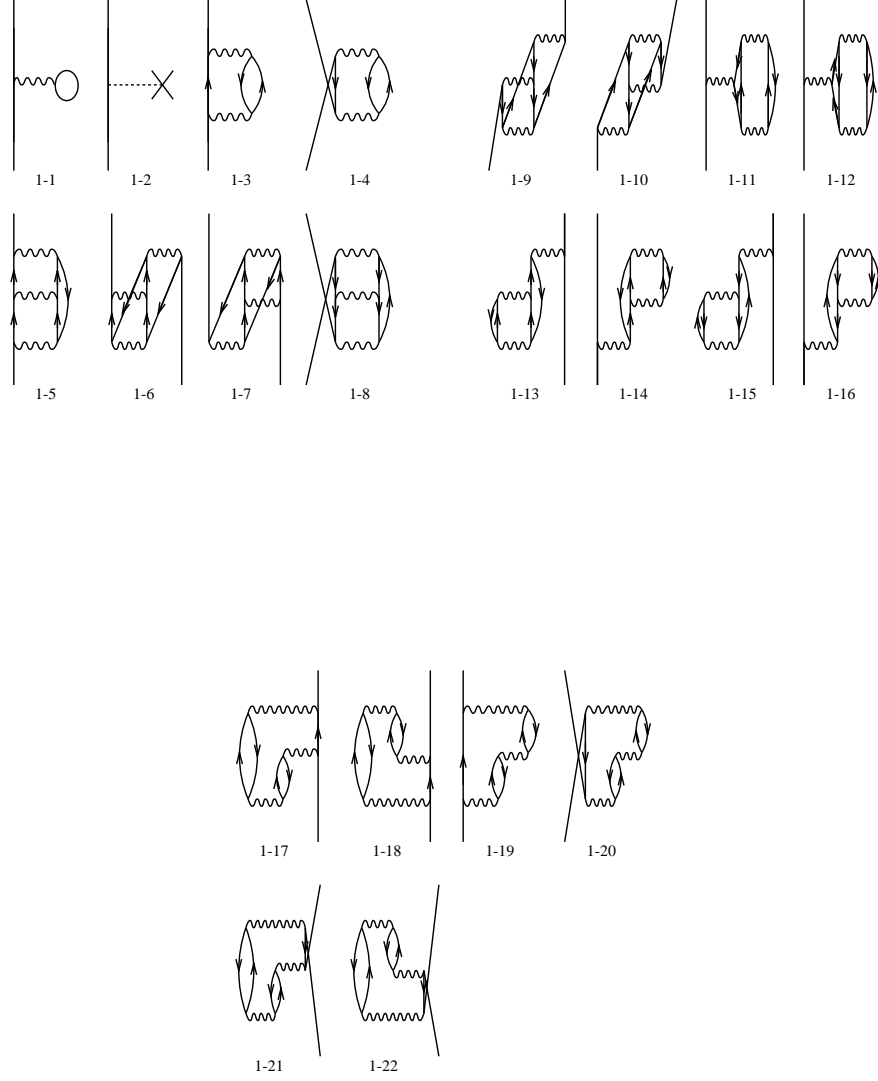


FIG. 1. One-body diagrams to third order in the interaction.

Diagram 1-22

$$-\sum_{ab}\sum_{ijk}\frac{\langle ap|\hat{v}|ik\rangle\langle bk|\hat{v}|jq\rangle\langle ij|\hat{v}|ab\rangle}{(\varepsilon_i+\varepsilon_k-\varepsilon_a-\varepsilon_p)(\varepsilon_q+\varepsilon_j+\varepsilon_i-\varepsilon_a-\varepsilon_b-\varepsilon_p)}.$$