3 Kutzelnigg-Mukherjee tensor notation

Notation 3.1. ***Kutzelnigg-Mukherjee tensor notation.*** In *Kutzelnigg-Mukherjee* (*KM*) *tensor notation*, creation operators are denoted using superscripts, $a^p \equiv a_p^\dagger$. Consequently, the one-particle and one-hole density matrices are written as $\gamma_q^p \equiv \langle\Phi|a^p a_q|\Phi\rangle$ and $\eta_p^q \equiv \langle\Phi|a_p a^q|\Phi\rangle$, respectively. The one- and two-electron integrals are also written with upper and lower indices: lower indices denote spin-orbitals in the bra and upper ones refer to spin-orbitals in the ket.

$$h_p^q \equiv \langle\psi_p|\hat{h}|\psi_q\rangle \qquad g_{pq}^{rs} \equiv \langle pq|rs\rangle \qquad \overline{g}_{pq}^{rs} \equiv \langle pq||rs\rangle \tag{3.1}$$

Vacuum-normal-ordered excitations are given the compact notation $a_{q_1\cdots q_m}^{p_1\cdots p_m} \equiv a^{p_1}\cdots a^{p_m}a_{q_m}\cdots a_{q_1}$ and Φ-normal-ordered excitations are written as $\tilde{a}_{q_1\cdots q_m}^{p_1\cdots p_m} \equiv \colon\!a^{p_1}\cdots a^{p_m}a_{q_m}\cdots a_{q_1}\!\colon$. Using upper and lower indices enables one to employ the *Einstein summation convention*, in which any index that appears twice in a product, once as a lower index and once as an upper one, is implicitly summed over. As an example, consider the electronic Hamiltonian as expressed in KM notation.

$$H_e = h_p^q a_q^p + \tfrac{1}{4}\overline{g}_{pq}^{rs}a_{rs}^{pq} = E_0 + H_c \qquad H_c = f_p^q\tilde{a}_q^p + \tfrac{1}{4}\overline{g}_{pq}^{rs}\tilde{a}_{rs}^{pq} \qquad E_0 \equiv h_p^q\gamma_q^p + \tfrac{1}{2}\overline{g}_{pr}^{qs}\gamma_q^p\gamma_s^r \qquad f_p^q \equiv h_p^q + \overline{g}_{pr}^{qs}\gamma_s^r \tag{3.2}$$

Here, E_0 is the Hartree-Fock reference energy, f_p^q denotes a matrix element of the Fock operator, and H_c denotes the correlation component of the Hamiltonian. More generally, if $\hat{v}$ is an *m-electron operator*, i.e. an operator that acts on m electronic coordinates, its second quantized form is expressed in KM notation as

$$\hat{v}\,|_{\mathcal{F}(\mathcal{H})} = \tfrac{1}{m!}v_{p_1\cdots p_m}^{q_1\cdots q_m}a_{q_1\cdots q_m}^{p_1\cdots p_m} \qquad v_{p_1\cdots p_m}^{q_1\cdots q_m} \equiv \int d(1\cdots m)\,\psi_{p_1}^*(1)\cdots\psi_{p_m}^*(m)\hat{v}(1,\ldots,m)\psi_{q_1}(1)\cdots\psi_{q_m}(m) \tag{3.3}$$

where $v_{p_1\cdots p_m}^{q_1\cdots q_m}$ is the *interaction tensor* of $\hat{v}$. Equivalently, $\hat{v}$ can also be expressed as

$$\hat{v}|_{\mathcal{F}(\mathcal{H})} = (\tfrac{1}{m!})^2\,\overline{v}_{p_1\cdots p_m}^{q_1\cdots q_m}a_{q_1\cdots q_m}^{p_1\cdots p_m} \qquad \overline{v}_{p_1\cdots p_m}^{q_1\cdots q_m} \equiv \sum_{\pi\in \mathrm{S}_m}\varepsilon_\pi v_{p_1}^{q_{\pi(1)}\cdots q_{\pi(m)}}{}_{\cdots p_m} \tag{3.4}$$

where $\overline{v}_{p_1\cdots p_m}^{q_1\cdots q_m}$ is an *antisymmetrized interaction tensor*. Ordinary interaction tensors are symmetric under simultaneous permutation of upper and lower indices, which is equivalent to changing integration variables in equation 3.3. Antisymmetrized interaction tensors allow for independent permutations of upper and lower indices, with a sign factor corresponding to the parity of the permutation. The same permutational symmetries are shared by the excitation operators

$$\tilde{a}_{q_1\cdots q_m}^{p_1\cdots p_m} = \varepsilon_\pi\tilde{a}_{q_1}^{p_{\pi(1)}\cdots p_{\pi(m)}}{}_{\cdots q_m} = \varepsilon_\pi\tilde{a}_{q_{\pi(1)}\cdots q_{\pi(m)}}^{p_1\quad\cdots p_m} = \tilde{a}_{q_{\pi(1)}\cdots q_{\pi(m)}}^{p_{\pi(1)}\cdots p_{\pi(m)}} \qquad \text{for all } \pi\in \mathrm{S}_m \tag{3.5}$$

since creation operators anticommute with each other, as do annihilation operators. Note also the following rearrangements

$$\tilde{a}_{q_1\cdots q_m}^{p_1\cdots p_m} = \colon\!a_{q_1}^{p_1}\cdots a_{q_m}^{p_m}\!\colon \qquad \colon\!a_{q_1\cdots q_m}^{p_1\cdots p_m}a_{s_1\cdots s_n}^{r_1\cdots r_n}\!\colon = \colon\!a_{q_1}^{p_1}\cdots a_{q_m}^{p_m}a_{s_1}^{r_1}\cdots a_{s_n}^{r_n}\!\colon = \tilde{a}_{q_1\cdots q_m s_1\cdots s_n}^{p_1\cdots p_m r_1\cdots r_n} \tag{3.6}$$

which follow from the fact that the normal-ordering mapping is antisymmetric with respect to its operator string.

Notation 3.2. ***Dot notation for contractions.*** To make the notation more flexible, we here augment the traditional KM notation with the following definitions of *particle* $\bullet$ *contractions* and *hole* $\circ$ *contractions*.[1]

$$a_{p^\bullet}a^{q^\bullet} \equiv \overbrace{a_p a^q} \qquad a^{q^\bullet}a_{p^\bullet} \equiv -\overbrace{a_p a^q} \qquad a^{q^\circ}a_{p^\circ} \equiv \overbrace{a^q a_p} \qquad a_{p^\circ}a^{q^\circ} \equiv -\overbrace{a^q a_p} \tag{3.7}$$

Note that $a_{q^\bullet}^{p^\bullet} = -\eta_q^p$ and $a_{q^\circ}^{p^\circ} = \gamma_q^p$. In vac-normal ordering, the hole contractions vanish and the particle contractions become Kronecker deltas. For multiply contracted strings, different contractions will be distinguished with repeated dots, $a_{p^{\bullet\bullet}}a^{p^{\bullet\bullet}}$, or dots with numbers, $a_{p^{\bullet 2}}a^{p^{\bullet 2}}$. This notation allows for normal ordered strings with contractions to keep all of the permutational symmetries shown in equations 3.5 and 3.6.

Example 3.1. Using notations 3.1 and 3.2, the Wick expansions for vacuum-normal single and double excitations in terms of Φ-normal ones look as follows. The signs are determined by pairing up contracted indices using eqs (3.5) and (3.6).

$$\begin{aligned} a_q^p &= \tilde{a}_q^p + \tilde{a}_{q^\circ}^{p^\circ} = \tilde{a}_q^p + \gamma_q^p \\ a_{rs}^{pq} &= \tilde{a}_{rs}^{pq} + \tilde{a}_{r^\circ s}^{p^\circ q} + \tilde{a}_{r\ s^\circ}^{p^\circ\ q} + \tilde{a}_{r^\circ s}^{p\ q^\circ} + \tilde{a}_{rs^\circ}^{pq^\circ} + \tilde{a}_{r^\circ s^{\circ\circ}}^{p^\circ q^{\circ\circ}} + \tilde{a}_{r^{\circ\circ}s^\circ}^{p^\circ\ q^{\circ\circ}} \\ &= \tilde{a}_{rs}^{pq} + \gamma_r^p\tilde{a}_s^q - \gamma_s^p\tilde{a}_r^q - \gamma_r^q\tilde{a}_s^p + \gamma_s^q\tilde{a}_r^p + \gamma_r^p\gamma_s^q - \gamma_s^p\gamma_r^q \end{aligned}$$

[1]The dot notation is borrowed from physics: `https://en.wikipedia.org/wiki/Wick's_theorem#Definition_of_contraction`

Definition 3.1. ***Index antisymmetrizers.*** Let $\hat{P}_{(p_1/\cdots/p_m)}$ denote an *index antisymmetrizer*, which antisymmetrizes a term with respect to $p_1, \ldots, p_m$ by summing over all permutations with an appropriate sign factor.

$$\hat{P}_{(p_1/\cdots/p_m)} t_{p_1 \cdots p_m} \equiv \sum_{\pi \in \mathrm{S}_m} \varepsilon_\pi t_{p_{\pi(1)} \cdots p_{\pi(m)}}$$

These operators can be expressed in terms of index transposition operators $\hat{p}_{pq}$, defined by $\hat{p}_{pq} t_{pq} \equiv t_{qp}$. For example,

$$\hat{P}_{(p/q)} \equiv 1 - \hat{p}_{pq} \qquad\qquad \hat{P}_{(p/q/r)} \equiv 1 - \hat{p}_{pq} - \hat{p}_{pr} - \hat{p}_{qr} + \hat{p}_{pq}\hat{p}_{qr} + \hat{p}_{pr}\hat{p}_{qr}$$

are the antisymmetrizers for two and three indices. More generally, antisymmetrizers of the form $\hat{P}_{(p_1 \cdots p_m / q_1 \cdots q_n / \cdots)}$ serve to antisymmetrize a term for which groups of indices are already antisymmetric. For example,

$$\hat{P}_{(p/qr)} = 1 - \hat{p}_{pq} - \hat{p}_{pr}$$

antisymmetrizes a term which is already antisymmetric with respect to q and r. These can be determined by generating permutations of (p, q, r) while treating q and r as indistinguishable.[2] In general, the antisymmetrizer $\hat{P}_{(R_1/\cdots/R_k)}$ involves a sum over $\frac{(|R_1|+\cdots+|R_k|)!}{|R_1|!\cdots|R_k|!}$ permutations, where each R_i is a set of indices and $|R_i|$ is its cardinality. To antisymmetrize multiple disjoint sets of indices, we use the compact notation $\hat{P}^{(X_1|\cdots|X_l)}_{(Y_1|\cdots|Y_m)} \equiv \hat{P}^{(X_1)} \cdots \hat{P}^{(X_l)} \hat{P}_{(Y_1)} \cdots \hat{P}_{(Y_m)}$. For example,

$$\hat{P}^{(p/q|r/st)}_{(u/v)} \equiv \hat{P}^{(p/q)} \hat{P}^{(r/st)} \hat{P}_{(u/v)} = (1 - \hat{p}^{pq})(1 - \hat{p}^{rs} - \hat{p}^{rt})(1 - \hat{p}_{uv}) \tag{3.8}$$

would antisymmetrize a term t^{pqrst}_{uv} with respect to (p, q), (u, v), and (r, s, t), assuming s and t are already antisymmetric.[3]

Example 3.2. Using index antisymmetrizers, the second Wick expansion in ex 3.1 can be expressed even more compactly.

$$a^{pq}_{rs} = \tilde{a}^{pq}_{rs} + \hat{P}^{(p/q)}_{(r/s)} \tilde{a}^{p^\circ q}_{r^\circ s} + \hat{P}_{(r/s)} \tilde{a}^{p^\circ q^{\circ\circ}}_{r^\circ s^{\circ\circ}} = \tilde{a}^{pq}_{rs} + \hat{P}^{(p/q)}_{(r/s)} \gamma^p_r \tilde{a}^{pq}_{rs} + \hat{P}_{(r/s)} \gamma^p_r \gamma^q_s$$

In general, this allows us to reduce Wick expansions to a sum over unique contraction "patterns", with the remaining contractions generated from these by index antisymmetrizers. The next two examples show how this works in practice.

Example 3.3. ***Derivation of CIS equations in KM notation.*** A programmable expression for the CI singles Hamiltonian matrix elements, $\langle \Phi^a_i | H_\mathrm{c} | \Phi^b_j \rangle$, can be derived in KM notation as follows.

$$\begin{aligned}
\langle \Phi | \tilde{a}^i_a \tilde{a}^p_q \tilde{a}^b_j | \Phi \rangle &= \colon\!\tilde{a}^{i^\circ}_{a^\bullet} a^{p^\bullet}_{q^\bullet} a^{b^{\bullet\bullet}}_{j^\circ}\!\colon + \colon\!\tilde{a}^{i^\circ}_{a^\bullet} a^{p^{\circ\circ}}_{q^\circ} a^{b^\bullet}_{j^{\circ\circ}}\!\colon = \gamma^i_j \eta^p_a \eta^b_q - \gamma^i_q \gamma^p_j \eta^b_a \\
\langle \Phi | \tilde{a}^i_a \tilde{a}^{pq}_{rs} \tilde{a}^b_j | \Phi \rangle &= \hat{P}^{(p/q)}_{(r/s)} \colon\!\tilde{a}^{i^\circ}_{a^\bullet} \tilde{a}^{p^\bullet q^{\circ\circ}}_{r^\circ s^{\bullet\bullet}} \tilde{a}^{b^{\bullet\bullet}}_{j^{\circ\circ}}\!\colon = \hat{P}^{(p/q)}_{(r/s)} \gamma^i_r \eta^p_a \gamma^q_j \eta^b_s \\
\implies \langle \Phi^a_i | H_\mathrm{c} | \Phi^b_j \rangle &= f^q_p \left(\gamma^i_j \eta^p_a \eta^b_q - \gamma^i_q \gamma^p_j \eta^b_a \right) + \tfrac{1}{4} \overline{g}^{rs}_{pq} \left(\hat{P}^{(p/q)}_{(r/s)} \gamma^i_r \eta^p_a \gamma^q_j \eta^b_s \right) = f^b_a \gamma^i_j - f^i_j \eta^b_a + \overline{g}^{ib}_{aj}
\end{aligned}$$

which simplifies to $\langle \Phi^a_i | H_\mathrm{c} | \Phi^b_j \rangle = f^b_a \delta^i_j - f^i_j \delta^b_a + \overline{g}^{ib}_{aj}$. Here, we have used the fact that $\tilde{a}^a_i = a^a_i$ and $\tilde{a}^i_a = a^i_a$.

Example 3.4. ***Derivation of CID equations in KM notation.*** Projecting the CI doubles Schrödinger equation, $H_\mathrm{c}\Psi = E_\mathrm{c}\Psi$ where $\Psi = (1 + \frac{1}{4} c^{kl}_{cd} \tilde{a}^{cd}_{kl})\Phi$, by Φ and Φ^{ab}_{ij} gives a system of linear equations

$$\begin{aligned}
E_\mathrm{c} &= \langle \Phi | H_\mathrm{c} (1 + \tfrac{1}{4} c^{kl}_{cd} \tilde{a}^{cd}_{kl}) | \Phi \rangle \qquad &\implies \qquad E_\mathrm{c} &= \tfrac{1}{4} \langle \Phi | H_c | \Phi^{cd}_{kl} \rangle c^{kl}_{cd} \\
E_\mathrm{c} c^{ij}_{ab} &= \langle \Phi^{ab}_{ij} | H_\mathrm{c} (1 + \tfrac{1}{4} c^{kl}_{cd} \tilde{a}^{cd}_{kl}) | \Phi \rangle \qquad &\implies \qquad E_\mathrm{c} c^{ij}_{ab} &= \langle \Phi^{ab}_{ij} | H_\mathrm{c} | \Phi \rangle + \tfrac{1}{4} \langle \Phi^{ab}_{ij} | H_\mathrm{c} | \Phi^{cd}_{kl} \rangle c^{kl}_{cd}
\end{aligned}$$

which can be simplified into programmable expressions as follows.

$$\begin{aligned}
\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^{cd}_{kl} | \Phi \rangle &= \hat{P}^{(p/q)}_{(r/s)} \gamma^p_k \gamma^q_l \eta^c_r \eta^d_s \\
\langle \Phi | \tilde{a}^{ij}_{ab} \tilde{a}^p_q \tilde{a}^{cd}_{kl} | \Phi \rangle &= \hat{P}^{(c/d)}_{(a/b|k/l)} \colon\!\tilde{a}^{i^{\circ 1} j^{\circ 2}}_{a^{\bullet 1} b^{\bullet 3}} \tilde{a}^{p^{\bullet 1}}_{q^{\bullet 2}} \tilde{a}^{c^{\bullet 2} d^{\bullet 3}}_{k^{\circ 1} l^{\circ 2}}\!\colon + \hat{P}^{(i/j|c/d)}_{(k/l)} \colon\!\tilde{a}^{i^{\circ 1} j^{\circ 3}}_{a^{\bullet 1} b^{\bullet 2}} \tilde{a}^{p^{\circ 2}}_{q^{\circ 1}} \tilde{a}^{c^{\bullet 1} d^{\bullet 2}}_{k^{\circ 2} l^{\circ 3}}\!\colon \\
&= \hat{P}^{(c/d)}_{(a/b|k/l)} \eta^p_a \eta^c_q \eta^d_b \gamma^i_k \gamma^j_l - \hat{P}^{(i/j|c/d)}_{(k/l)} \gamma^i_q \gamma^p_k \gamma^j_l \eta^c_a \eta^d_b \\
\langle \Phi | \tilde{a}^{ij}_{ab} \tilde{a}^{pq}_{rs} \tilde{a}^{cd}_{kl} | \Phi \rangle &= \hat{P}^{(c/d)}_{(a/b|k/l)} \colon\!\tilde{a}^{i^{\circ 1} j^{\circ 2}}_{a^{\bullet 1} b^{\bullet 2}} \tilde{a}^{p^{\bullet 1} q^{\bullet 2}}_{r^{\bullet 3} s^{\bullet 4}} \tilde{a}^{c^{\bullet 3} d^{\bullet 4}}_{k^{\circ 1} l^{\circ 2}}\!\colon + \hat{P}^{(i/j|c/d)}_{(k/l)} \colon\!\tilde{a}^{i^{\circ 1} j^{\circ 2}}_{a^{\bullet 1} b^{\bullet 2}} \tilde{a}^{p^{\circ 3} q^{\circ 4}}_{r^{\circ 1} s^{\circ 2}} \tilde{a}^{c^{\bullet 1} d^{\bullet 2}}_{k^{\circ 3} l^{\circ 4}}\!\colon + \hat{P}^{(p/q|i/j|c/d)}_{(r/s|k/l|a/b)} \colon\!\tilde{a}^{i^{\circ 1} j^{\circ 3}}_{a^{\bullet 1} b^{\bullet 3}} \tilde{a}^{p^{\circ 2} q^{\bullet 1}}_{r^{\circ 1} s^{\bullet 2}} \tilde{a}^{c^{\bullet 2} d^{\bullet 3}}_{k^{\circ 2} l^{\circ 3}}\!\colon \\
&= \hat{P}^{(c/d)}_{(a/b|k/l)} \eta^p_a \eta^q_b \eta^c_r \eta^d_s \gamma^i_k \gamma^j_l + \hat{P}^{(i/j|c/d)}_{(k/l)} \gamma^i_r \gamma^j_s \gamma^p_k \gamma^q_l \eta^c_a \eta^d_b - \hat{P}^{(p/q|i/j|c/d)}_{(r/s|k/l|a/b)} \gamma^i_r \gamma^p_k \gamma^j_l \eta^q_a \eta^c_s \eta^d_b
\end{aligned}$$

$$\implies \qquad E_\mathrm{c} = \tfrac{1}{4} \overline{g}^{cd}_{kl} c^{kl}_{cd} \qquad\qquad E_\mathrm{c} c^{ij}_{ab} = \overline{g}^{ij}_{ab} + \hat{P}_{(a/b)} f^c_a c^{ij}_{cb} - \hat{P}^{(i/j)} f^i_k c^{kj}_{ab} + \tfrac{1}{2} \overline{g}^{cd}_{ab} c^{ij}_{cd} + \tfrac{1}{2} \overline{g}^{ij}_{kl} c^{kl}_{ab} + \hat{P}^{(i/j)}_{(a/b)} \overline{g}^{ic}_{ak} c^{jk}_{bc}$$

[2] For example, (p, q, r) and (p, r, q) would be treated as equivalent permutations. Only one of these is used, and it doesn't matter which one. Note however that, in determining the sign factor for a permutation, q and r are again treated as distinct.

[3] For some more examples, see p. 324 of Shavitt and Bartlett, *Many-Body Methods in Chemistry and Physics* (2009).