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 $\tilde{a}_{q_1\cdots q_m}^{p_1\cdots p_m} \equiv \{\!\!\{a^{p_1}\cdots a^{p_m}a_{q_m}\cdots a_{q_1}\}\!\!\}$. 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.

$$H = h_p^q a_q^p + \tfrac{1}{4}\overline{g}_{pq}^{rs}a_{rs}^{pq} = E_{\text{ref}} + H_{\text{c}} \qquad H_{\text{c}} = f_p^q\tilde{a}_q^p + \tfrac{1}{4}\overline{g}_{pq}^{rs}\tilde{a}_{rs}^{pq} \qquad E_{\text{ref}} \equiv h_p^q\gamma_q^p + \tfrac{1}{2}\overline{g}_{pr}^{qs}\gamma_q^p\gamma_s^r \qquad f_p^q \equiv h_p^q + \overline{g}_{pr}^{qs}\gamma_s^r \tag{3.2}$$

Here, E_{ref} 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

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

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

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

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

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

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).

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

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

Definition 3.1. ***Riffle shuffle permutations.*** Let S_R be the *symmetric group on* $R \equiv (r_1, \ldots, r_k)$, comprising all $k!$ permutations of this tuple. For each integer composition[2] $(k_1, \ldots, k_m)$ of k, the $(k_1, \ldots, k_m)$-*shuffles of* R partition the tuple into blocks $R_1 \cup \cdots \cup R_m$ of the form $R_i \equiv (r_{h_i+1}, \ldots, r_{h_i+k_i})$ with $h_i \equiv \sum_{j=1}^{i-1} k_j$ and interleave them in all possible ways. The cardinality of this subset $\mathrm{S}_R^{(k_1,\ldots,k_m)} \subseteq \mathrm{S}_R$ is given by the following multinomial coefficient

$$|\mathrm{S}_R^{(k_1,\ldots,k_m)}| \equiv \frac{k!}{k_1! \cdots k_m!} \tag{3.8}$$

since for each shuffle there are $k_1! \cdots k_m!$ permutations in S_R derived by permuting the elements within each block. These are termed *riffle shuffle permutations*,[3] by analogy with the process of cutting and interleaving a deck of cards.

Definition 3.2. ***Index antisymmetrizers.*** Let $\hat{P}_{(r_1/\cdots/r_k)}$ be the *full antisymmetrizer* for the indices in R.[4] [5] More generally, let $\hat{P}_{(R_1/\cdots/R_m)}$ be a *reduced antisymmetrizer*, which antisymmetrizes a term in R that it is already antisymmetric in each block, R_i. Reduced antisymmetrization is achieved by summing over riffle shuffles.

$$\hat{P}_{(R_1/\cdots/R_m)} \equiv \sum_{\pi}^{\mathrm{S}_R^{(k_1,\ldots,k_m)}} \varepsilon_\pi \hat{\pi} \qquad\qquad \hat{\pi}\, t_{r_1 \cdots r_k} \equiv t_{\pi(r_1)\cdots\pi(r_k)} \tag{3.9}$$

To antisymmetrize multiple disjoint sets of indices, we use the compact notation $\hat{P}_{(Y_1|\cdots|Y_m)}^{(X_1|\cdots|X_l)} \equiv \hat{P}^{(X_1)} \cdots \hat{P}^{(X_l)} \hat{P}_{(Y_1)} \cdots \hat{P}_{(Y_m)}$, where each X_i or Y_i stands for a reduced antisymmetrizer argument $R_1/\cdots/R_m$ for a different set of indices.

Example 3.2. Permutation operators $\hat{\pi}$ can be written as products of transpositions $(pq)t_{pq} \equiv t_{qp}$. In this notation,

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

are the unique antisymmetrizers for two and three indices. Note that $\hat{P}_{(p/qr)}\hat{P}_{(q/r)} = \hat{P}_{(p/q/r)}$, which is an immediate consequence of the definition of the reduced antisymmetrizer.

Example 3.3. Using index antisymmetrizers, the second Wick expansion in ex 3.1 can be expressed even more compactly.

$$a_{rs}^{pq} = \tilde{a}_{rs}^{pq} + \hat{P}_{(r/s)}^{(p/q)} \tilde{a}_{r^\circ s}^{p^\circ q} + \hat{P}_{(r/s)} \tilde{a}_{r^\circ s^{\circ\circ}}^{p^\circ q^{\circ\circ}} = \tilde{a}_{rs}^{pq} + \hat{P}_{(r/s)}^{(p/q)} \gamma_r^p \tilde{a}_{rs}^{pq} + \hat{P}_{(r/s)} \gamma_r^p \gamma_s^q$$

Note that permuting p and q in the second term, for example, is equivalent to "moving the contraction dot" from one to the other, since the excitation operators are antisymmetric in their upper and lower indices: $(pq)\tilde{a}_{r^\circ s}^{p^\circ q} = -\tilde{a}_{r^\circ s}^{q^\circ p} = \tilde{a}_{r^\circ s}^{p\ q^\circ}$. 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 3.4. Reduced antisymmetrizers come into play in the Wick expansion of a triple excitation operator.

$$a_{stu}^{pqr} = \tilde{a}_{stu}^{pqr} + \hat{P}_{(s/tu)}^{(p/qr)} \tilde{a}_{s^\circ tu}^{p^\circ qr} + \hat{P}_{(st/u)}^{(p/q/r)} \tilde{a}_{s^\circ t^{\circ\circ} u}^{p^\circ q^{\circ\circ} r} + \hat{P}^{(p/q/r)} \tilde{a}_{s^\circ t^{\circ\circ} u^{\circ\circ\circ}}^{p^\circ q^{\circ\circ} r^{\circ\circ\circ}} \tag{3.10}$$

The permutation factors are chosen as follows. In the second term, permutations of qr an tu are omitted because they do not produce unique contractions. In the third term, we can include permutations of either pq or st but not both. Otherwise, we would double-count terms like $\tilde{a}_{s^\circ t^{\circ\circ} u}^{p^\circ q^{\circ\circ} r}$ by also including $\tilde{a}_{s^{\circ\circ} t^\circ u}^{p^{\circ\circ} q^\circ r}$, which represents the same contraction. The same reasoning applies to the last term, where we can either antisymmetrize pqr or stu.

Example 3.5. ***Derivation of CIS equations in KM notation.*** A programmable expression for the CI singles Hamiltonian matrix elements, $\langle \Phi_i^a | H_c | \Phi_j^b \rangle$, can be derived in KM notation as follows.

$$\begin{aligned}
\langle \Phi | \tilde{a}_a^i \tilde{a}_q^p \tilde{a}_j^b | \Phi \rangle &= \vdots a_{a^\bullet}^{i^\circ} a_{q^{\bullet\bullet}}^{p^\bullet} a_{j^\circ}^{b^{\bullet\bullet}} \vdots + \vdots a_{a^\bullet}^{i^\circ} a_{q^\circ}^{p^{\circ\circ}} a_{j^{\circ\circ}}^{b^\bullet} \vdots = \gamma_j^i \eta_a^p \eta_q^b - \gamma_q^i \gamma_j^p \eta_a^b \\
\langle \Phi | \tilde{a}_a^i \tilde{a}_{rs}^{pq} \tilde{a}_j^b | \Phi \rangle &= \hat{P}_{(r/s)}^{(p/q)} \vdots a_{a^\bullet}^{i^\circ} a_{r^\circ s^{\bullet\bullet}}^{p^\bullet q^{\circ\circ}} a_{j^{\circ\circ}}^{b^{\bullet\bullet}} \vdots = \hat{P}_{(r/s)}^{(p/q)} \gamma_r^i \eta_a^p \gamma_j^q \eta_s^b \\
\implies \langle \Phi_i^a | H_c | \Phi_j^b \rangle &= f_p^q \left(\gamma_j^i \eta_a^p \eta_q^b - \gamma_q^i \gamma_j^p \eta_a^b \right) + \tfrac{1}{4} \overline{g}_{pq}^{rs} \left(\hat{P}_{(r/s)}^{(p/q)} \gamma_r^i \eta_a^p \gamma_j^q \eta_s^b \right) = f_a^b \gamma_j^i - f_j^i \eta_a^b + \overline{g}_{aj}^{ib}
\end{aligned}$$

which simplifies to $\langle \Phi_i^a | H_c | \Phi_j^b \rangle = f_a^b \delta_j^i - f_j^i \delta_a^b + \overline{g}_{aj}^{ib}$. Here, we have used the fact that $\tilde{a}_i^a = a_i^a$ and $\tilde{a}_a^i = a_a^i$.

[2] See `https://en.wikipedia.org/wiki/Composition_(combinatorics)`

[3] See `https://en.wikipedia.org/wiki/Riffle_shuffle_permutation`

[4] Note that we are borrowing some definitions from def 3.1, such as R and R_i.

[5] For example, we can express the position-space Slater determinant $\Phi_{(p_1 \cdots p_n)}(1, \ldots, n)$ as $\frac{1}{\sqrt{n!}} \hat{P}_{(p_1/\cdots/p_n)} \psi_{p_1}(1) \cdots \psi_{p_n}(n)$.

Example 3.6. ***Derivation of CID equations in KM notation.*** Projecting the CI doubles Schrödinger equation, $H_\mathrm{c}\Psi = E_\mathrm{c}\Psi$ where $\Psi = (1 + \frac{1}{4}c_{cd}^{kl}\tilde{a}_{kl}^{cd})\Phi$, by Φ and Φ_{ij}^{ab} gives a system of linear equations

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

which can be simplified into programmable expressions as follows.

$$\begin{aligned} \langle\Phi|\tilde{a}_{rs}^{pq}\tilde{a}_{kl}^{cd}|\Phi\rangle &= \hat{P}_{(r/s)}^{(p/q)}\gamma_k^p\gamma_l^q\eta_r^c\eta_s^d \\ \langle\Phi|\tilde{a}_{ab}^{ij}\tilde{a}_q^p\tilde{a}_{kl}^{cd}|\Phi\rangle &= \hat{P}_{(a/b|k/l)}^{(c/d)}\vdots a_{a^{\bullet_1}b^{\bullet_3}}^{i^{\circ_1}j^{\circ_2}}a_{q^{\bullet_2}}^{p^{\bullet_1}}a_{k^{\circ_1}l^{\circ_2}}^{c^{\bullet_2}d^{\bullet_3}}\vdots + \hat{P}_{(k/l)}^{(i/j|c/d)}\vdots a_{a^{\bullet_1}b^{\bullet_2}}^{i^{\circ_1}j^{\circ_3}}a_{q^{\circ_1}}^{p^{\circ_2}}a_{k^{\circ_2}l^{\circ_3}}^{c^{\bullet_1}d^{\bullet_2}}\vdots \\ &= \hat{P}_{(a/b|k/l)}^{(c/d)}\eta_a^p\eta_q^c\eta_b^d\gamma_k^i\gamma_l^j - \hat{P}_{(k/l)}^{(i/j|c/d)}\gamma_q^i\gamma_k^p\gamma_l^j\eta_a^c\eta_b^d \\ \langle\Phi|\tilde{a}_{ab}^{ij}\tilde{a}_{rs}^{pq}\tilde{a}_{kl}^{cd}|\Phi\rangle &= \hat{P}_{(a/b|k/l)}^{(c/d)}\vdots a_{a^{\bullet_1}b^{\bullet_2}}^{i^{\circ_1}j^{\circ_2}}a_{r^{\bullet_3}s^{\bullet_4}}^{p^{\bullet_1}q^{\bullet_2}}a_{k^{\circ_1}l^{\circ_2}}^{c^{\bullet_3}d^{\bullet_4}}\vdots + \hat{P}_{(k/l)}^{(i/j|c/d)}\vdots a_{a^{\bullet_1}b^{\bullet_2}}^{i^{\circ_1}j^{\circ_2}}a_{r^{\circ_1}s^{\circ_2}}^{p^{\circ_3}q^{\circ_4}}a_{k^{\circ_3}l^{\circ_4}}^{c^{\bullet_1}d^{\bullet_2}}\vdots + \hat{P}_{(r/s|k/l|a/b)}^{(p/q|i/j|c/d)}\vdots a_{a^{\bullet_1}b^{\bullet_3}}^{i^{\circ_1}j^{\circ_3}}a_{r^{\circ_1}s^{\bullet_2}}^{p^{\circ_2}q^{\bullet_1}}a_{k^{\circ_2}l^{\circ_3}}^{c^{\bullet_2}d^{\bullet_3}}\vdots \\ &= \hat{P}_{(a/b|k/l)}^{(c/d)}\eta_a^p\eta_b^q\eta_r^c\eta_s^d\gamma_k^i\gamma_l^j + \hat{P}_{(k/l)}^{(i/j|c/d)}\gamma_r^i\gamma_s^j\gamma_k^p\gamma_l^q\eta_a^c\eta_b^d - \hat{P}_{(r/s|k/l|a/b)}^{(p/q|i/j|c/d)}\gamma_r^i\gamma_k^p\gamma_l^j\eta_a^q\eta_s^c\eta_b^d \end{aligned}$$

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