Multipartite entanglement and correlation

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Structure [2, 3, 4]

- state vector: $|\psi\rangle \in \mathcal{H}$ (normalized)
- pure state: $\pi = |\psi\rangle\langle\psi| \in \mathcal{P}$
- mixed state (of an ensemble): $\varrho = \sum_j p_j \pi_j \in \mathcal{D} = \operatorname{Conv}\mathcal{P}$

Level 0: subsystems

- system: $L = [n] = \{1, 2, \dots, n\}$
- subsystem: $X \subseteq L$, then $\mathcal{H}_X$, $\mathcal{P}_X$, $\mathcal{D}_X$ — Boolean lattice structure: $P_0 = 2^L$

Level I: partitions [3, 4, 5, 6, 7]

- partitions of the system: $\xi = \{X_1, X_2, \dots, X_{|\xi|}\} \equiv X_1|X_2|\dots|X_{|\xi|} \in \Pi(L)$
- refinement: $\upsilon \preceq \xi$ def.: $\forall Y \in \upsilon, \exists X \in \xi : Y \subseteq X$ — lattice structure: $P_{\mathrm{I}} = \Pi(L)$
- ξ-uncorrelated states: $\mathcal{D}_{\xi\text{-unc}} = \{\otimes_{X\in\xi}\varrho_X\}$ — $\upsilon \preceq \xi \iff \mathcal{D}_{\upsilon\text{-unc}} \subseteq \mathcal{D}_{\xi\text{-unc}}$
- ξ-separable states: $\mathcal{D}_{\xi\text{-sep}} = \operatorname{Conv}\mathcal{D}_{\xi\text{-unc}}$ — $\upsilon \preceq \xi \iff \mathcal{D}_{\upsilon\text{-sep}} \subseteq \mathcal{D}_{\xi\text{-sep}}$

Level II: multiple partitions [3, 4, 5, 6]

- down-sets of partitions: $\boldsymbol{\xi} = \{\xi_1, \xi_2, \dots, \xi_{|\boldsymbol{\xi}|}\} \subseteq P_{\mathrm{I}}$ (closed downwards w.r.t. $\preceq$)
- partial order: $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi}$ def.: $\boldsymbol{\upsilon} \subseteq \boldsymbol{\xi}$ — lattice structure: $P_{\mathrm{II}} = \mathcal{O}_\downarrow(P_{\mathrm{I}}) \setminus \{\emptyset\}$
- $\boldsymbol{\xi}$-uncorrelated states: $\mathcal{D}_{\boldsymbol{\xi}\text{-unc}} = \cup_{\xi\in\boldsymbol{\xi}}\mathcal{D}_{\xi\text{-unc}}$ — $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi} \iff \mathcal{D}_{\boldsymbol{\upsilon}\text{-unc}} \subseteq \mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$
- $\boldsymbol{\xi}$-separable states: $\mathcal{D}_{\boldsymbol{\xi}\text{-sep}} = \operatorname{Conv}\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$ — $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi} \iff \mathcal{D}_{\boldsymbol{\upsilon}\text{-sep}} \subseteq \mathcal{D}_{\boldsymbol{\xi}\text{-sep}}$
- spec.: k-partitionability and k'-producibility (chains)

$$\boldsymbol{\mu}_k = \{\mu \in P_{\mathrm{I}} \mid |\mu| \geq k\}, \qquad \boldsymbol{\nu}_{k'} = \{\nu \in P_{\mathrm{I}} \mid \forall N \in \nu : |N| \leq k'\}$$

k-partitionably unc. and k'-producibly unc.: $\mathcal{D}_{k\text{-part unc}} = \mathcal{D}_{\boldsymbol{\mu}_k\text{-unc}}$, $\mathcal{D}_{k'\text{-prod unc}} = \mathcal{D}_{\boldsymbol{\nu}_{k'}\text{-unc}}$

k-partitionably sep. and k'-producibly sep.: $\mathcal{D}_{k\text{-part sep}} = \mathcal{D}_{\boldsymbol{\mu}_k\text{-sep}}$, $\mathcal{D}_{k'\text{-prod sep}} = \mathcal{D}_{\boldsymbol{\nu}_{k'}\text{-sep}}$

Level III: entanglement classes [2, 4]

- up-sets of down-sets of partitions: $\underline{\boldsymbol{\xi}} = \{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_{|\underline{\boldsymbol{\xi}}|}\} \subseteq P_{\mathrm{II}}$ (closed upw. w.r.t. $\preceq$)
- partial order: $\underline{\boldsymbol{\upsilon}} \preceq \underline{\boldsymbol{\xi}}$ def.: $\underline{\boldsymbol{\upsilon}} \subseteq \underline{\boldsymbol{\xi}}$ — lattice structure: $P_{\mathrm{III}} = \mathcal{O}_\uparrow(P_{\mathrm{II}}) \setminus \{\emptyset\}$
- partial correlation classes [2]: all the possible intersections of $\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$

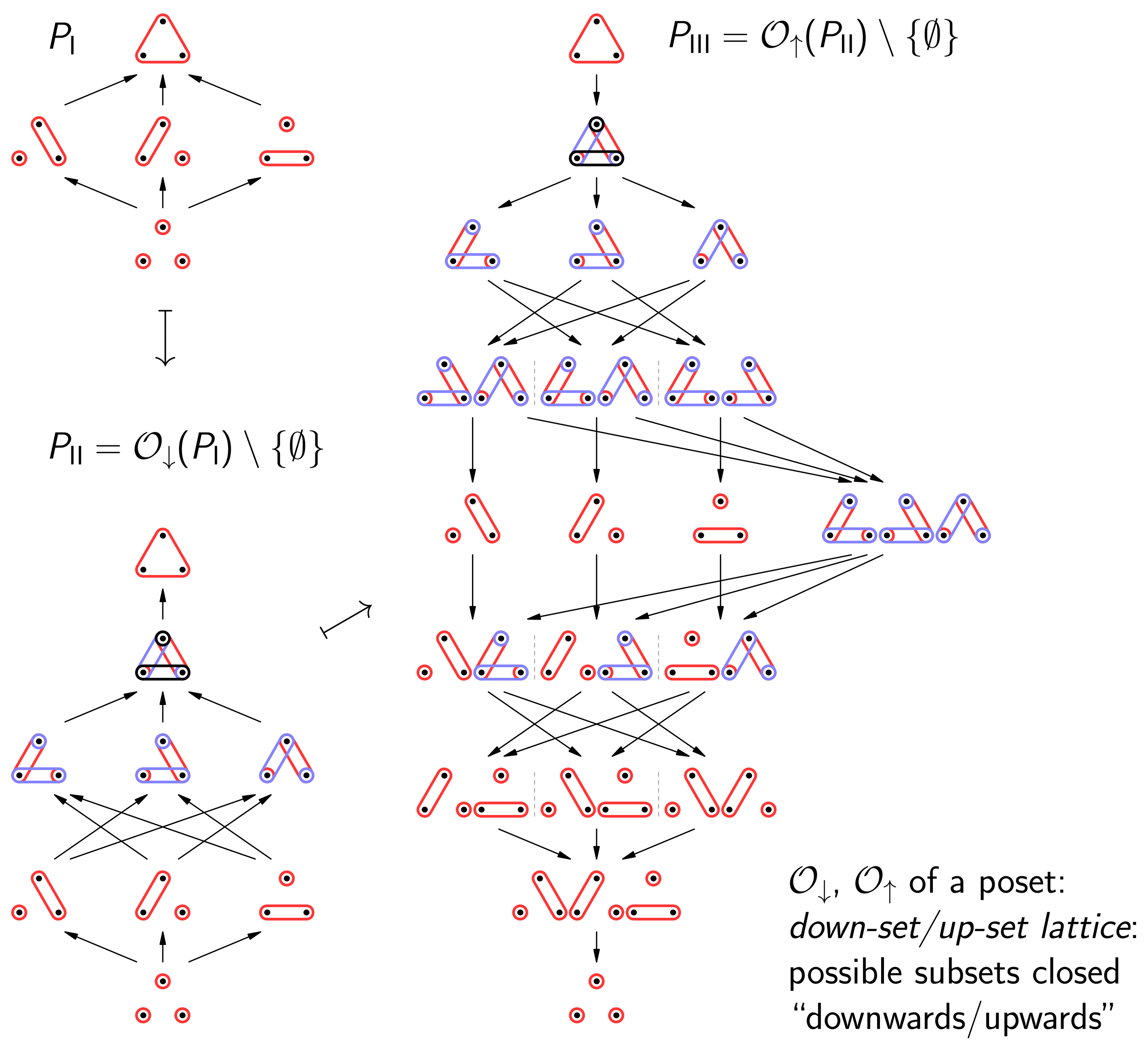
$$\mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-unc}} = \bigcap_{\boldsymbol{\xi}\notin\underline{\boldsymbol{\xi}}} \overline{\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}} \cap \bigcap_{\boldsymbol{\xi}\in\underline{\boldsymbol{\xi}}} \mathcal{D}_{\boldsymbol{\xi}\text{-unc}} \qquad \text{for principals: } \underline{\boldsymbol{\xi}} = \uparrow\{\downarrow\{\xi\}\}$$

- LO convertibility: if $\exists\varrho \in \mathcal{C}_{\underline{\boldsymbol{\upsilon}}\text{-unc}}$, $\exists\Lambda$ LO map such that $\Lambda(\varrho) \in \mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-unc}}$ then $\underline{\boldsymbol{\upsilon}} \preceq \underline{\boldsymbol{\xi}}$
- partial separability classes [4]: all the possible intersections of $\mathcal{D}_{\boldsymbol{\xi}\text{-sep}}$

$$\mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-sep}} = \bigcap_{\boldsymbol{\xi}\notin\underline{\boldsymbol{\xi}}} \overline{\mathcal{D}_{\boldsymbol{\xi}\text{-sep}}} \cap \bigcap_{\boldsymbol{\xi}\in\underline{\boldsymbol{\xi}}} \mathcal{D}_{\boldsymbol{\xi}\text{-sep}} \qquad \text{for all } \underline{\boldsymbol{\xi}} \text{ (conjecture)}$$

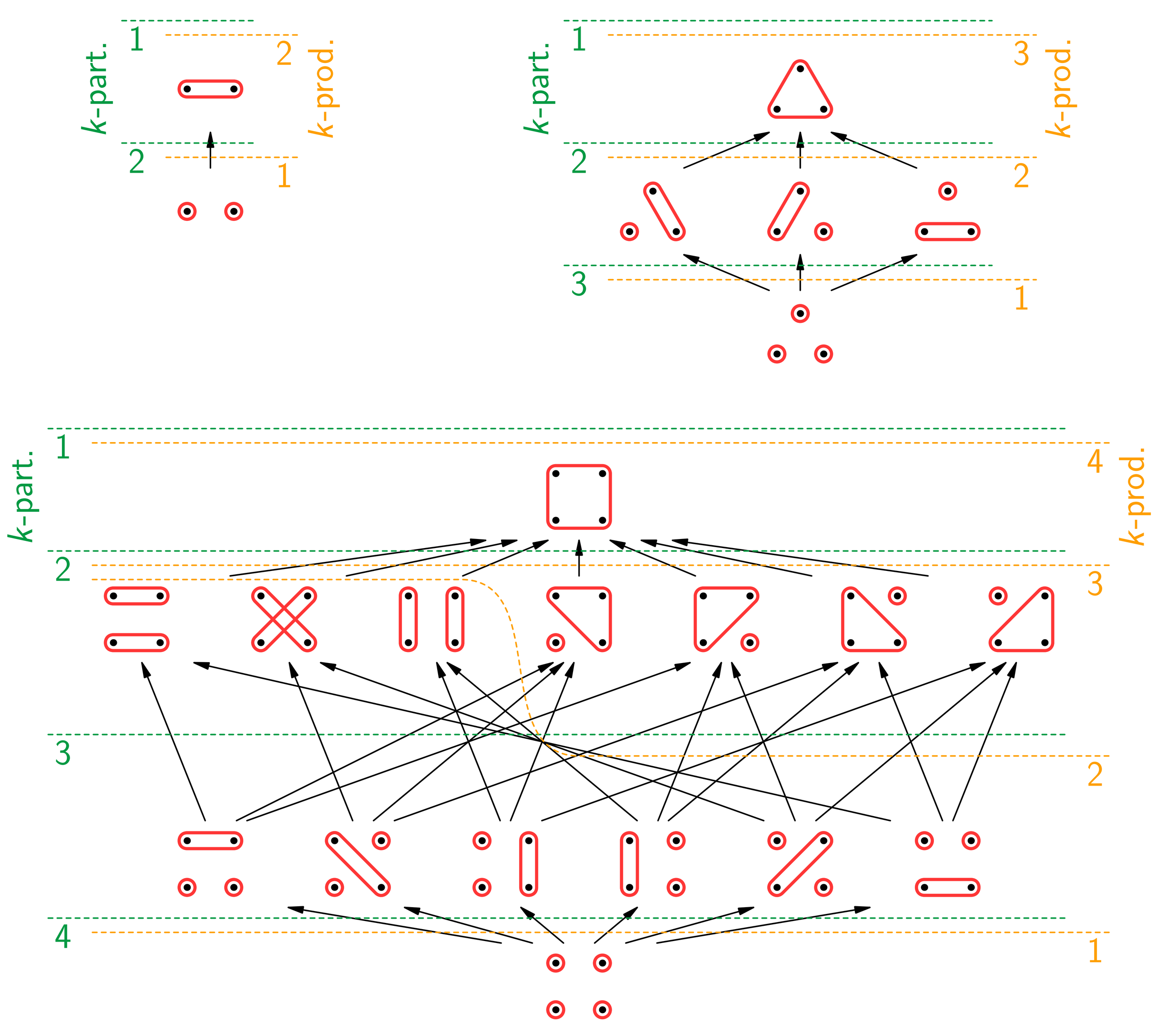
- LOCC convertibility: if $\exists\varrho \in \mathcal{C}_{\underline{\boldsymbol{\upsilon}}\text{-sep}}$, $\exists\Lambda$ LOCC map such that $\Lambda(\varrho) \in \mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-sep}}$ then $\underline{\boldsymbol{\upsilon}} \preceq \underline{\boldsymbol{\xi}}$

Illustrations: Structure for $n = 3$ [4]



$\mathcal{O}_\downarrow$, $\mathcal{O}_\uparrow$ of a poset: *down-set/up-set lattice*: possible subsets closed "downwards/upwards"

Illustrations: k-partitionability and k'-producibility for $n = 2, 3, 4$ [1, 3, 4]



Quantification [3, 4, 5]

- mixedness: von Neumann entropy $S(\varrho) = -\operatorname{tr}\varrho\ln\varrho$
- distinguishability: relative entropy $D(\varrho\|\sigma) = \operatorname{tr}\varrho(\ln\varrho - \ln\sigma)$

Level I: partitions [3, 4]

- ξ-correlation (ξ-mutual information):

$$C_\xi(\varrho) = \min_{\sigma\in\mathcal{D}_{\xi\text{-unc}}} D(\varrho\|\sigma) = \sum_{X\in\xi} S(\varrho_X) - S(\varrho)$$

- ξ-entanglement (for pure states), ξ-entanglement of formation (for mixed states):

$$E_\xi(\pi) = C_\xi|_{\mathcal{P}}(\pi), \qquad E_\xi(\varrho) = \min\Big\{\sum_i p_i E_\xi(\pi_i) \;\Big|\; \sum_i p_i\pi_i = \varrho\Big\}$$

strong entanglement monotone: not increasing on average w.r.t. selective LOCC

- faithful: $C_\xi(\varrho) = 0 \iff \varrho \in \mathcal{D}_{\xi\text{-unc}}$, $E_\xi(\varrho) = 0 \iff \varrho \in \mathcal{D}_{\xi\text{-sep}}$
- multipartite monotone: $\upsilon \preceq \xi \iff C_\upsilon \geq C_\xi$, $E_\upsilon \geq E_\xi$

Level II: multiple partitions [3, 4]

- $\boldsymbol{\xi}$-correlation:

$$C_{\boldsymbol{\xi}}(\varrho) = \min_{\sigma\in\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}} D(\varrho\|\sigma) = \min_{\xi\in\boldsymbol{\xi}} C_\xi(\varrho)$$

- $\boldsymbol{\xi}$-entanglement (for pure states), $\boldsymbol{\xi}$-entanglement of formation (for mixed states):

$$E_{\boldsymbol{\xi}}(\pi) = C_{\boldsymbol{\xi}}|_{\mathcal{P}}(\pi), \qquad E_{\boldsymbol{\xi}}(\varrho) = \min\Big\{\sum_i p_i E_{\boldsymbol{\xi}}(\pi_i) \;\Big|\; \sum_i p_i\pi_i = \varrho\Big\}$$

strong entanglement monotone: not increasing on average w.r.t. selective LOCC

- faithful: $C_{\boldsymbol{\xi}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$, $E_{\boldsymbol{\xi}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{\boldsymbol{\xi}\text{-sep}}$
- multipartite monotone: $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi} \iff C_{\boldsymbol{\upsilon}} \geq C_{\boldsymbol{\xi}}$, $E_{\boldsymbol{\upsilon}} \geq E_{\boldsymbol{\xi}}$
- spec.: k-partitionability and k'-producibility
  k-partitionability correlation and k'-producibility correlation:

$$C_{k\text{-part}}(\varrho) = C_{\boldsymbol{\mu}_k}(\varrho) = \min_{|\mu|\geq k} C_\mu(\varrho), \qquad C_{k'\text{-prod}}(\varrho) = C_{\boldsymbol{\nu}_{k'}}(\varrho) = \min_{\forall N\in\nu:|N|\leq k'} C_\nu(\varrho)$$

faithful: $C_{k\text{-part}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{k\text{-part unc}}$, $C_{k'\text{-prod}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{k'\text{-prod unc}}$

multipartite monotone: $k < l \iff C_{k\text{-part}} \leq C_{l\text{-part}}$, $C_{k\text{-prod}} \geq C_{l\text{-prod}}$

k-partitionability entanglement of form. and k'-producibility entanglement of form.:

$$E_{k\text{-part}}(\varrho) = E_{\boldsymbol{\mu}_k}(\varrho), \qquad E_{k'\text{-prod}}(\varrho) = E_{\boldsymbol{\nu}_{k'}}(\varrho)$$

faithful: $E_{k\text{-part}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{k\text{-part sep}}$, $E_{k'\text{-prod}}(\varrho) = 0 \iff \varrho \in \mathcal{D}_{k'\text{-prod sep}}$

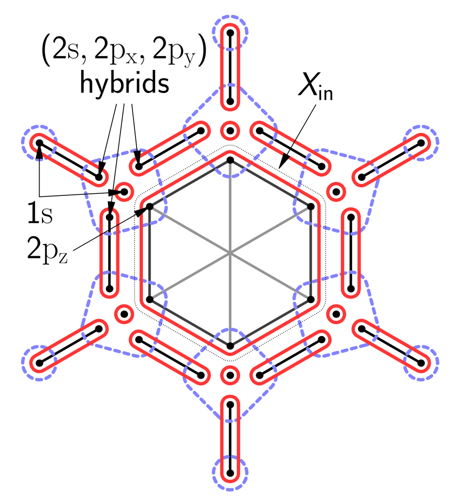
multipartite monotone: $k < l \iff E_{k\text{-part}} \leq E_{l\text{-part}}$, $E_{k\text{-prod}} \geq E_{l\text{-prod}}$

Examples: Multipartite correlations in molecules [1, 3]

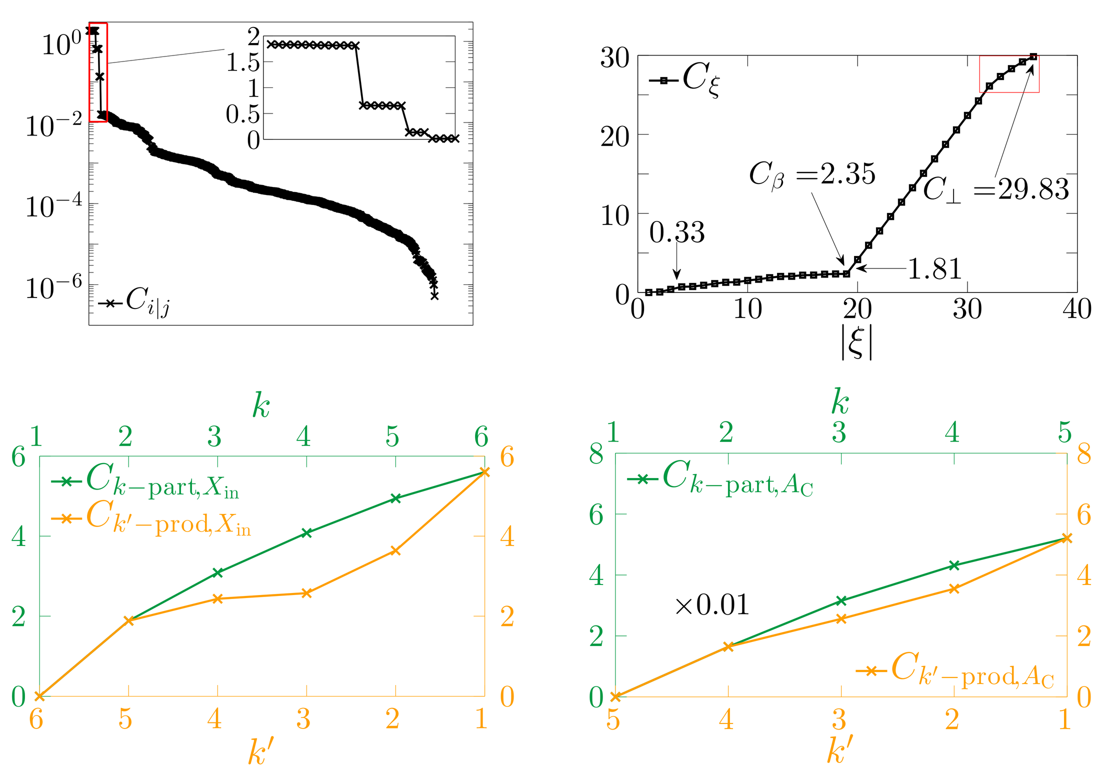
"atoms": $\alpha = A_1|A_2|\dots|A_{|\alpha|}$, "bonds": $\beta = B_1|B_2|\dots|B_{|\beta|}$

$$\sum_{A\in\alpha} C_{\perp,A}(\varrho_A) + C_\alpha(\varrho) = \sum_{B\in\beta} C_{\perp,B}(\varrho_B) + C_\beta(\varrho) = C_\perp(\varrho)$$

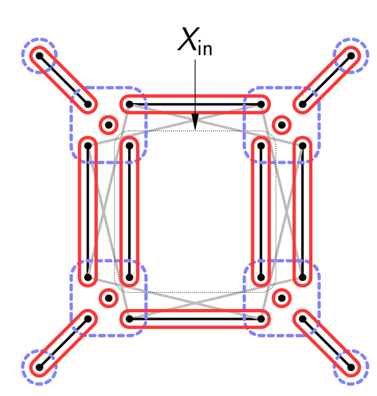
C_6H_6 (benzene):



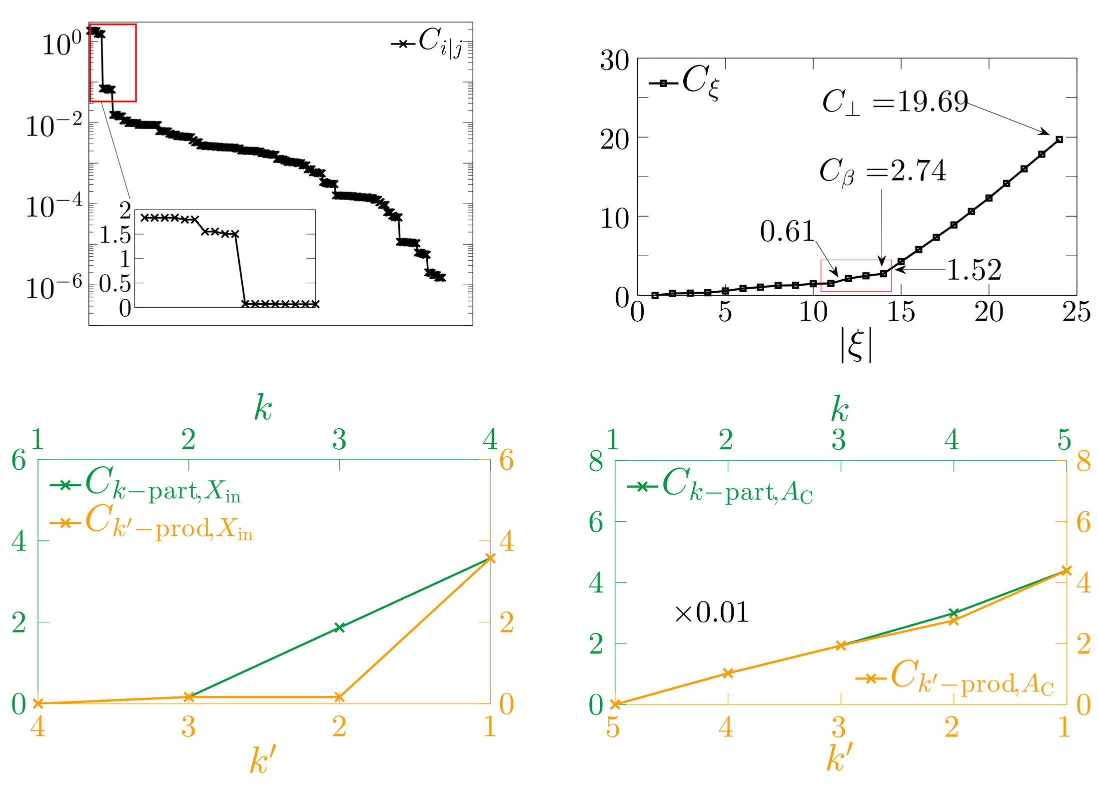
$C_\alpha = 29.52$, $C_\beta = 2.35$



C_4H_4 (cyclobutadiene):



$C_\alpha = 19.51$, $C_\beta = 2.74$



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