Supporting Information

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1. Full tables

Tables I and II show all the numerical results displayed in the Figures of the main manuscript.

Table I. Full results number of measurement groups needed for different reduction methods. In Scenario I and II we considered the number of steps that achieved the lowest error. Free H_6 refers to randomized molecule geometries and the values correspond to mean and standard deviation of the sample.

Method	Linear H_4	Square H_4	Linear H_6	Circular H_6	Free H_6	Linear H_8
Original H	361	357	1623	1795	1382±265	3985
Pauli-grouping						
LF	28	21	90	91	74±15	154
RLF	19	22	60	64	54±8	111
SI	19	19	68	77	64±9	114
Fermionic-grouping						
LR	10	11	22	22	20±2	33
FFF-LR	10	11	22	22	20±2	33
This work						
Scenario I	9	9	9	15	45±38	6
Scenario II	9	9	9	15	12±20	6

Table II. Full results number of measurement needed for different reduction methods. Every number is multiplied by $\times 10^4$. Free H_6 refers to randomized molecule geometries and the values correspond to mean and standard deviation of the sample.

Method	Linear H_4	Square H_4	Linear H_6	Circular H_6	Free H_6	Linear H_8
Pauli-grouping						
LF	11.89	6.41	19.10	35.10	16.06±6.36	26.88
RLF	4.99	9.94	22.24	27.08	16.60±6.65	25.89
SI	3.48	2.77	3.58	4.27	4.60±2.15	3.60
Fermionic-grouping						
LR	119.96	167.26	164.59	268.19	253.73±64.54	237.93
FFF-LR	3.89	155.24	3.74	258.04	16.13±7.57	3.17
This work						
Scenario I	2.28	2.44	2.55	3.17	5.69±4.57	2.60
Scenario II	2.19	2.44	2.35	3.17	4.94±4.78	2.48

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GLOSSARY

LF: Large First [1]
RLF: Recursive Largest First [1]
SI: Sorted Insertion [2, 3]
LR: Low-rank decomposition [4, 5]
FFF-LR: Fluid Fermionic Fragments [6]

2. Visualization of HCB elements

The operators α_k, β_{kl}, γ_{kl} and δ_{kl} presented in the main manuscript account for multiple creation and destruction fermionic operators with all possible spin combinations. In Figure 1 we display a visual representation of all the terms that one needs to take into consideration and why we can interpret them as paired-electrons or quasi-bosonic particle creation and destruction operators. In each of the four operators we end up with two terms which provide the same contribution. The $\frac{1}{2}$ coefficient in the Hamiltonian definition takes care of this repetition.

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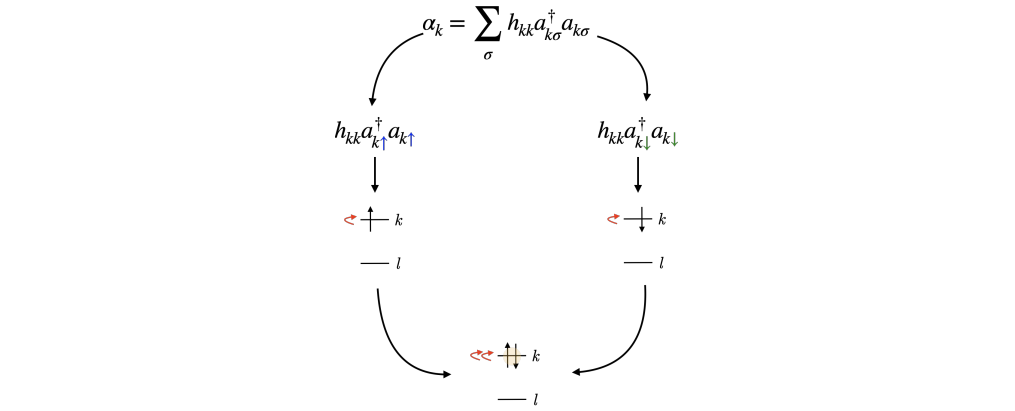
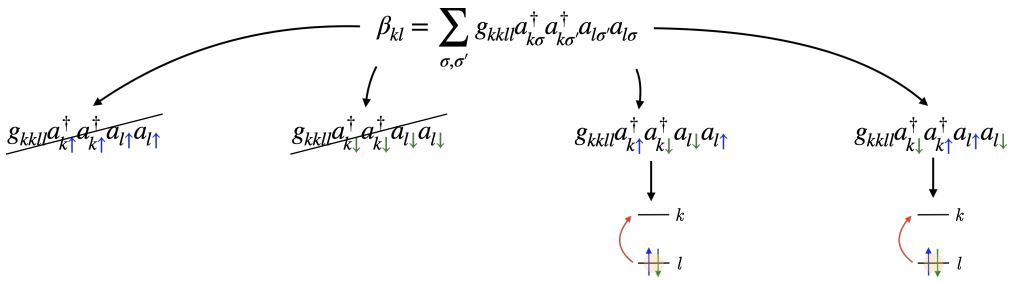
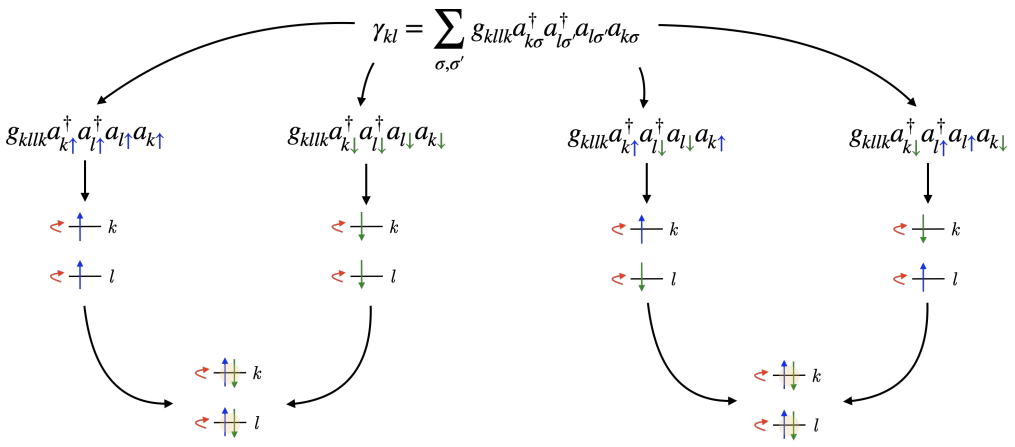


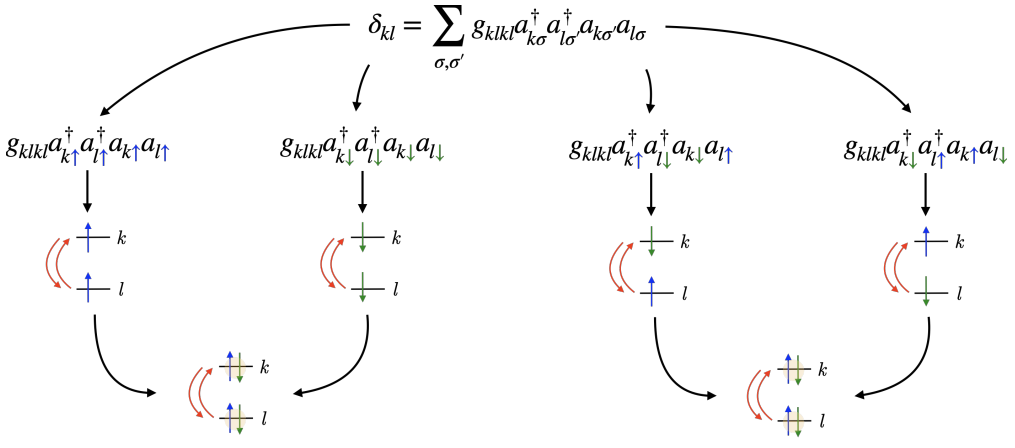
(a) α_k



(b) β_{kl}



(c) γ_{kl}



(d) δ_{kl}

Figure 1. Visualization of HCB elements. Each operator is expanded in all the possible spin combinations. These are then visually represented to explicit the paired-electrons, or quasi-bosonic particles, interpretation. The first and second terms stemming from β_{kl} with all coherent spins are not allowed due to fermionic operators commutativity properties.