

hybrid methods in seniority space

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for the Gemini¹

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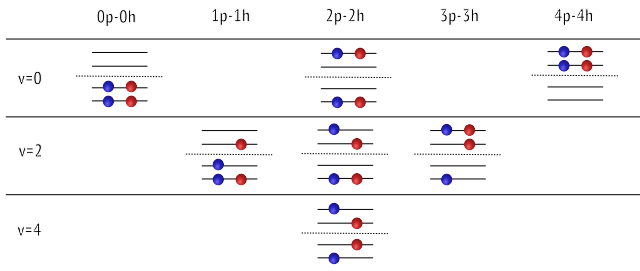
CECAM Valence Bond
27-30 March 2017

Hierarchy by Seniority

- Hamiltonian can be reordered wrt **seniority** ($\nu = 0, 2, 4$)

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{ik}^{v=0} V_{iikk} a_i^\dagger a_i^\dagger a_{\bar{k}} a_k + \sum_{i \neq j, k}^{v=2} V_{ijkk} (a_i^\dagger a_j^\dagger a_{\bar{k}} a_k + h.c.) + \dots$$

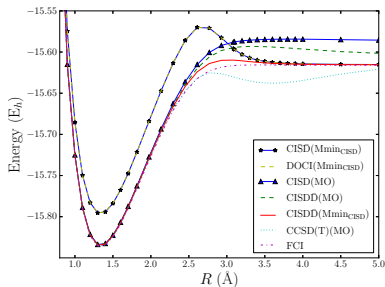
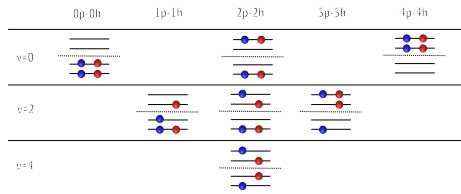
- seniority**: number of particles *not* coupled pairwise together
- pair creation $S_i^\dagger = a_i^\dagger a_{\bar{i}}^\dagger$ & annihilation $S_i = a_{\bar{i}} a_i$



Open-shell correlations: truncated CI

hybrid methods

- DOCI for **static** correlations
- CISD for **dynamics** correlations
- orbital optimization

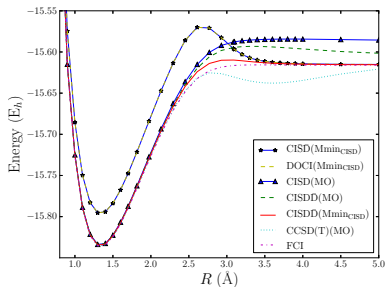
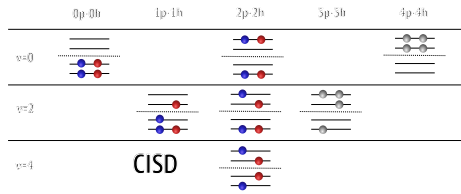


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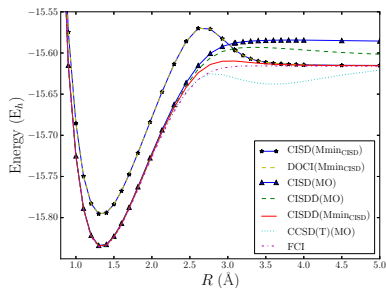
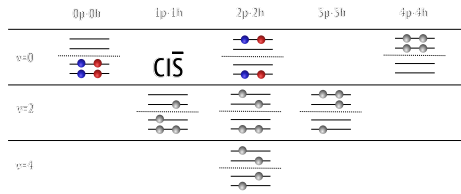



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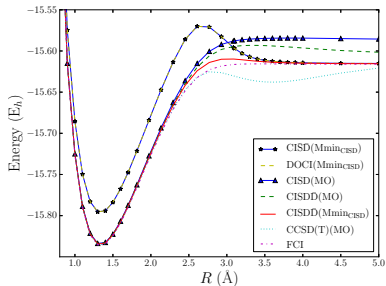
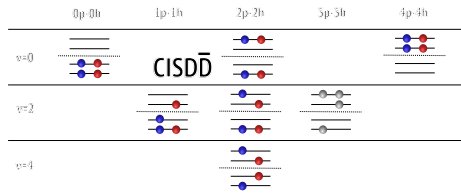


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